



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 06:45 PM EST

PDB ID : 8DJK
EMDB ID : EMD-27460
Title : HMGCR-UBIAD1 Complex State 2
Authors : Chen, H.; Qi, X.; Li, X.
Deposited on : 2022-06-30
Resolution : 3.33 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

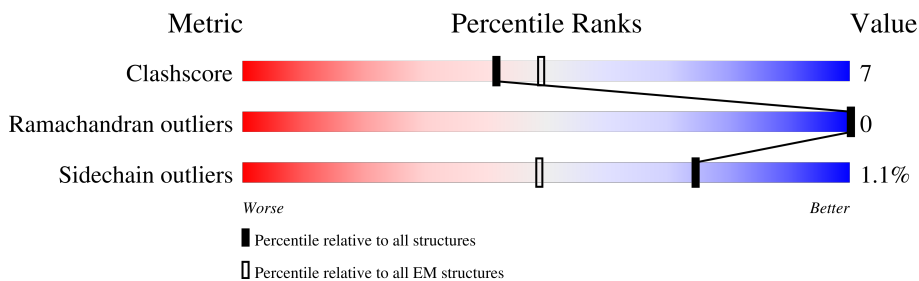
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	364	
2	B	301	
3	C	120	
4	L	214	
5	H	232	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	Y01	A	401	X	-	-	-
6	Y01	A	402	X	-	-	-
6	Y01	A	403	X	-	-	-
6	Y01	A	404	X	-	-	-
6	Y01	A	405	X	-	-	-
6	Y01	B	402	X	-	-	-
7	AJP	A	406	X	-	X	-
7	AJP	B	401	X	-	X	-

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7091 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	245	1930	1261	318	333	18	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P00347
A	-6	ASP	-	expression tag	UNP P00347
A	-5	TYR	-	expression tag	UNP P00347
A	-4	LYS	-	expression tag	UNP P00347
A	-3	ASP	-	expression tag	UNP P00347
A	-2	ASP	-	expression tag	UNP P00347
A	-1	ASP	-	expression tag	UNP P00347
A	0	ASP	-	expression tag	UNP P00347
A	1	LYS	-	expression tag	UNP P00347
A	89	ARG	LYS	conflict	UNP P00347
A	248	ARG	LYS	conflict	UNP P00347

- Molecule 2 is a protein called UbiA prenyltransferase domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	281	2152	1431	338	374	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	38	MET	-	initiating methionine	UNP G3IEF0
B	39	ALA	-	expression tag	UNP G3IEF0
B	40	SER	-	expression tag	UNP G3IEF0
B	102	SER	ASN	conflict	UNP G3IEF0

- Molecule 3 is a protein called Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	120	944	585	171	186	2	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	264	ALA	-	expression tag	UNP P0ABE7
C	265	ARG	-	expression tag	UNP P0ABE7
C	266	ARG	-	expression tag	UNP P0ABE7
C	267	LEU	-	expression tag	UNP P0ABE7
C	268	ALA	-	expression tag	UNP P0ABE7
C	273	TRP	MET	conflict	UNP P0ABE7
C	368	ILE	HIS	conflict	UNP P0ABE7
C	372	LEU	-	expression tag	UNP P0ABE7
C	373	GLU	-	expression tag	UNP P0ABE7
C	374	ARG	-	expression tag	UNP P0ABE7
C	375	ALA	-	expression tag	UNP P0ABE7
C	376	ARG	-	expression tag	UNP P0ABE7
C	377	SER	-	expression tag	UNP P0ABE7
C	378	THR	-	expression tag	UNP P0ABE7
C	379	LEU	-	expression tag	UNP P0ABE7
C	380	GLN	-	expression tag	UNP P0ABE7
C	381	LYS	-	expression tag	UNP P0ABE7
C	382	GLU	-	expression tag	UNP P0ABE7
C	383	VAL	-	expression tag	UNP P0ABE7

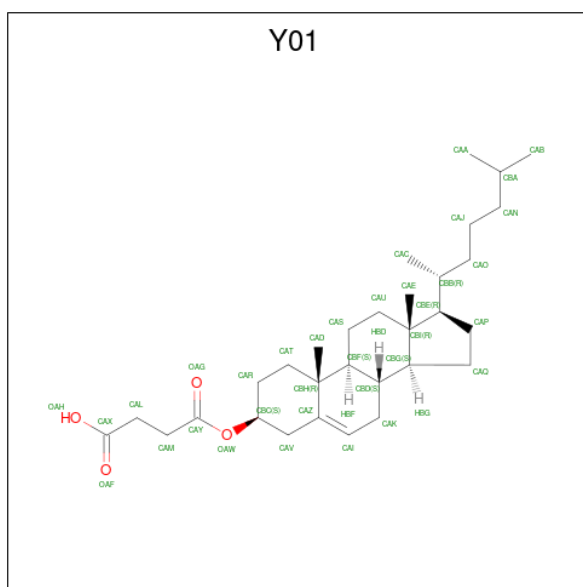
- Molecule 4 is a protein called Fab 15B2 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	106	808	504	136	166	2	0	0

- Molecule 5 is a protein called Fab 15B2 Heavy Chain.

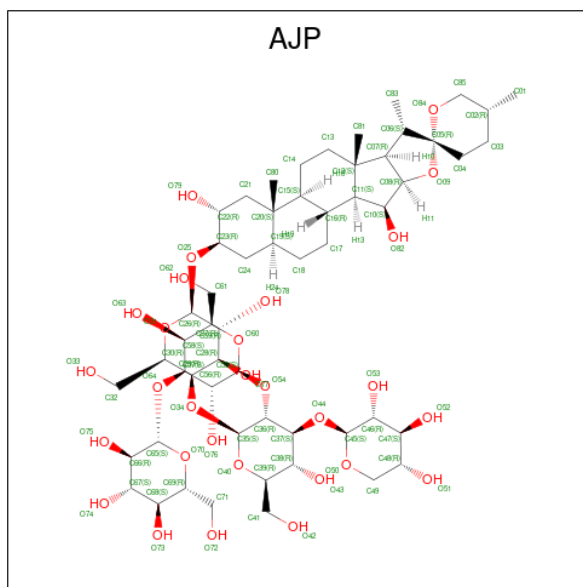
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	H	118	930	587	160	178	5	0	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	175	155	20	0
6	A	1	175	155	20	0
6	A	1	175	155	20	0
6	A	1	175	155	20	0
6	A	1	175	155	20	0
6	B	1	35	31	4	0

- Molecule 7 is Digitonin (three-letter code: AJP) (formula: $C_{56}H_{92}O_{29}$).

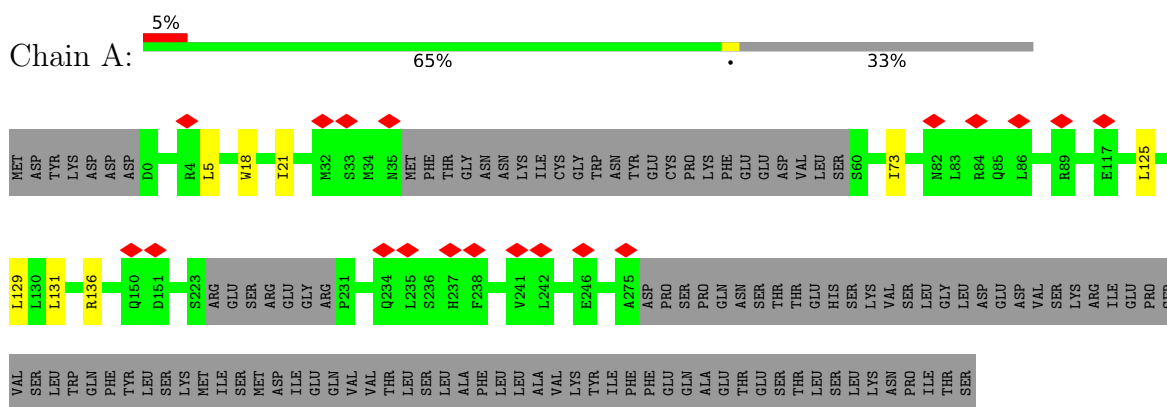


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			74	50	24	
7	B	1	Total	C	O	0
			43	33	10	

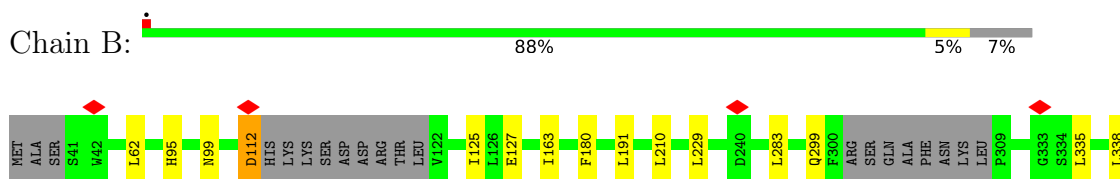
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

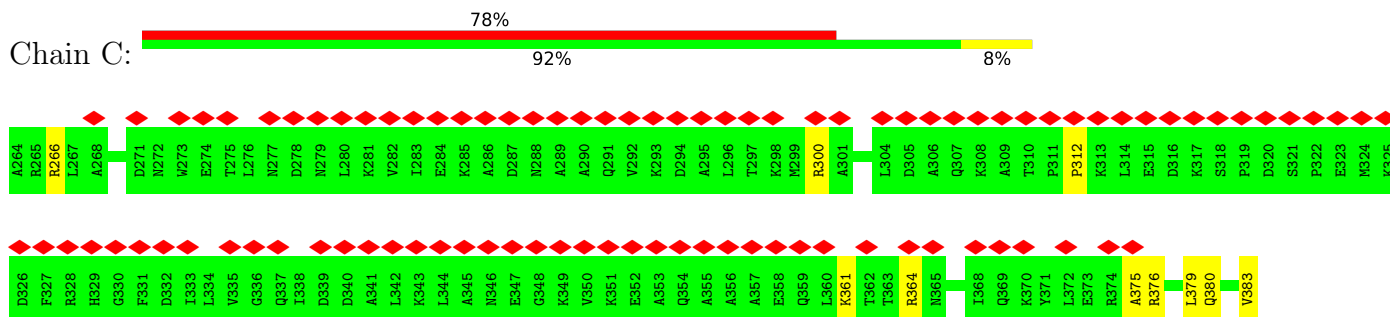
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 2: UbiA prenyltransferase domain-containing protein 1

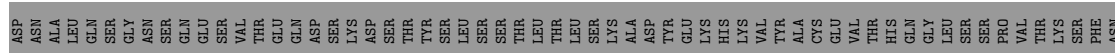
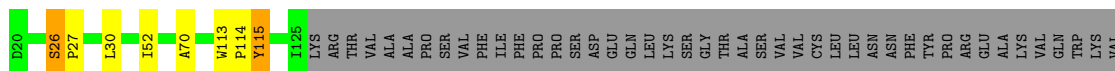


- Molecule 3: Soluble cytochrome b562

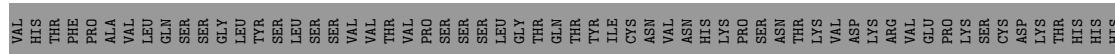
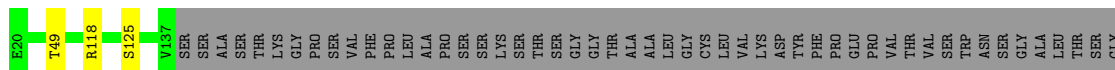


- Molecule 4: Fab 15B2 Light Chain





• Molecule 5: Fab 15B2 Heavy Chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.993	Depositor
Minimum map value	-3.296	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.351	Depositor
Map size (\AA)	269.44, 269.44, 269.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.842, 0.842, 0.842	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AJP, Y01

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/1969	0.58	0/2665
2	B	0.43	0/2204	0.57	0/3005
3	C	0.43	0/954	0.59	0/1283
4	L	0.54	2/826 (0.2%)	0.73	3/1121 (0.3%)
5	H	0.36	0/953	0.54	0/1285
All	All	0.43	2/6906 (0.0%)	0.59	3/9359 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	113	TRP	C-N	8.11	1.49	1.34
4	L	113	TRP	C-O	6.22	1.35	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	26	SER	C-N-CD	6.78	142.63	128.40
4	L	114	PRO	N-CA-C	-5.99	96.53	112.10
4	L	26	SER	N-CA-C	5.80	126.67	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	26	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1930	0	1988	6	0
2	B	2152	0	2225	12	0
3	C	944	0	960	12	0
4	L	808	0	769	6	0
5	H	930	0	892	2	0
6	A	175	0	235	24	0
6	B	35	0	48	8	0
7	A	74	0	0	22	0
7	B	43	0	0	21	0
All	All	7091	0	7117	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:401:AJP:C16	7:B:401:AJP:C15	1.76	1.64
6:A:404:Y01:CBH	6:A:404:Y01:CBF	1.75	1.62
6:A:401:Y01:CBF	6:A:401:Y01:CBH	1.75	1.60
6:B:402:Y01:CBH	6:B:402:Y01:CBF	1.75	1.60
6:A:405:Y01:CBH	6:A:405:Y01:CBF	1.76	1.58
7:A:406:AJP:C15	7:A:406:AJP:C16	1.77	1.58
7:B:401:AJP:C12	7:B:401:AJP:C11	1.81	1.54
7:A:406:AJP:C12	7:A:406:AJP:C11	1.82	1.53
7:A:406:AJP:C02	7:A:406:AJP:C01	1.96	1.44
7:B:401:AJP:C02	7:B:401:AJP:C01	1.97	1.42
7:A:406:AJP:C08	7:A:406:AJP:C07	2.00	1.39
7:B:401:AJP:C08	7:B:401:AJP:C07	2.01	1.39
7:B:401:AJP:O09	7:B:401:AJP:C05	1.80	1.29
7:A:406:AJP:O09	7:A:406:AJP:C05	1.79	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:401:AJP:C11	7:B:401:AJP:C07	2.28	1.12
7:A:406:AJP:C08	7:A:406:AJP:C05	2.33	1.06
7:B:401:AJP:C08	7:B:401:AJP:C05	2.34	1.06
7:A:406:AJP:C11	7:A:406:AJP:C07	2.34	1.04
2:B:299:GLN:O	3:C:383:VAL:HG21	1.69	0.91
4:L:27:PRO:HG3	4:L:30:LEU:HD12	1.58	0.86
4:L:27:PRO:CG	4:L:30:LEU:HD12	2.10	0.81
2:B:299:GLN:NE2	3:C:379:LEU:HD13	1.95	0.81
7:B:401:AJP:C15	7:B:401:AJP:C17	2.59	0.80
7:B:401:AJP:C07	7:B:401:AJP:C10	2.58	0.80
7:A:406:AJP:C15	7:A:406:AJP:C11	2.59	0.80
7:A:406:AJP:C01	7:A:406:AJP:C03	2.54	0.79
7:A:406:AJP:C07	7:A:406:AJP:C10	2.59	0.79
7:B:401:AJP:C08	7:B:401:AJP:C06	2.62	0.77
7:A:406:AJP:C16	7:A:406:AJP:C20	2.62	0.76
7:B:401:AJP:C12	7:B:401:AJP:C08	2.57	0.76
7:B:401:AJP:C16	7:B:401:AJP:C20	2.63	0.76
7:B:401:AJP:C01	7:B:401:AJP:C03	2.58	0.76
7:B:401:AJP:C01	7:B:401:AJP:C85	2.60	0.76
7:B:401:AJP:C11	7:B:401:AJP:C81	2.64	0.76
7:A:406:AJP:C08	7:A:406:AJP:C06	2.65	0.75
7:A:406:AJP:C01	7:A:406:AJP:C85	2.63	0.74
6:A:405:Y01:CBF	6:A:405:Y01:CAT	2.65	0.74
6:A:404:Y01:CBF	6:A:404:Y01:CAT	2.66	0.74
7:A:406:AJP:C12	7:A:406:AJP:C08	2.56	0.74
3:C:376:ARG:HD2	3:C:376:ARG:C	2.10	0.72
3:C:380:GLN:HA	3:C:380:GLN:OE1	1.89	0.72
6:A:401:Y01:CBF	6:A:401:Y01:CAT	2.68	0.72
7:B:401:AJP:C15	7:B:401:AJP:C11	2.64	0.71
6:B:402:Y01:CBF	6:B:402:Y01:CAT	2.68	0.71
6:A:401:Y01:CBF	6:A:401:Y01:CAZ	2.66	0.71
6:B:402:Y01:CBF	6:B:402:Y01:CAZ	2.68	0.71
7:A:406:AJP:C11	7:A:406:AJP:C81	2.68	0.70
6:A:404:Y01:CBF	6:A:404:Y01:CAZ	2.69	0.70
2:B:299:GLN:NE2	3:C:379:LEU:CD1	2.54	0.70
7:A:406:AJP:C11	7:A:406:AJP:C13	2.70	0.68
7:B:401:AJP:C11	7:B:401:AJP:C13	2.72	0.63
6:A:403:Y01:HAC1	6:A:403:Y01:HAU1	1.81	0.63
6:A:404:Y01:CBH	6:A:404:Y01:CAS	2.72	0.62
7:A:406:AJP:O09	7:A:406:AJP:C04	2.42	0.61
6:A:405:Y01:CBH	6:A:405:Y01:CAS	2.76	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:405:Y01:CBF	6:A:405:Y01:CAD	2.76	0.60
6:A:403:Y01:HAC1	6:A:403:Y01:CAU	2.31	0.60
7:B:401:AJP:O09	7:B:401:AJP:C04	2.42	0.60
6:A:401:Y01:CBH	6:A:401:Y01:CBD	2.74	0.60
4:L:27:PRO:HG2	4:L:30:LEU:HD12	1.86	0.57
6:A:401:Y01:CBH	6:A:401:Y01:CAS	2.77	0.57
6:B:402:Y01:CBH	6:B:402:Y01:CAS	2.75	0.57
7:A:406:AJP:C16	7:A:406:AJP:C80	2.83	0.57
2:B:191:LEU:HD12	2:B:229:LEU:HD22	1.87	0.56
6:A:401:Y01:CBF	6:A:401:Y01:CAD	2.78	0.56
7:B:401:AJP:C12	7:B:401:AJP:C10	2.80	0.56
1:A:5:LEU:HB3	6:A:402:Y01:HAQ2	1.89	0.55
2:B:95:HIS:CE1	2:B:99:ASN:HD21	2.25	0.54
2:B:299:GLN:HG3	3:C:379:LEU:HD11	1.88	0.54
2:B:112:ASP:N	2:B:112:ASP:OD1	2.41	0.54
1:A:136:ARG:CZ	7:A:406:AJP:O77	2.57	0.53
4:L:115:TYR:CD1	4:L:115:TYR:N	2.77	0.52
6:A:401:Y01:CBH	6:A:401:Y01:HBF	2.18	0.52
6:A:404:Y01:CBF	6:A:404:Y01:CAD	2.79	0.52
4:L:115:TYR:N	4:L:115:TYR:HD1	2.08	0.52
6:A:405:Y01:CBH	6:A:405:Y01:HBF	2.18	0.51
7:B:401:AJP:C16	7:B:401:AJP:C12	2.78	0.51
1:A:136:ARG:NH1	7:A:406:AJP:O77	2.43	0.51
7:A:406:AJP:C16	7:A:406:AJP:C12	2.78	0.50
6:B:402:Y01:CBF	6:B:402:Y01:CAD	2.78	0.49
6:A:405:Y01:CBH	6:A:405:Y01:CBD	2.77	0.49
2:B:299:GLN:HE21	3:C:379:LEU:CD1	2.23	0.49
7:B:401:AJP:C08	7:B:401:AJP:C81	2.90	0.48
3:C:312:PRO:HD2	3:C:375:ALA:HB1	1.95	0.48
3:C:376:ARG:HD2	3:C:376:ARG:O	2.13	0.48
6:B:402:Y01:CBH	6:B:402:Y01:CBD	2.76	0.48
3:C:266:ARG:HG3	3:C:380:GLN:NE2	2.30	0.46
6:B:402:Y01:HAC1	6:B:402:Y01:HAU2	1.98	0.45
7:A:406:AJP:C08	7:A:406:AJP:C81	2.95	0.45
1:A:125:LEU:O	1:A:129:LEU:HG	2.17	0.45
1:A:73:ILE:HG23	1:A:131:LEU:HD12	1.97	0.45
2:B:163:ILE:HD11	2:B:210:LEU:HD21	1.99	0.44
4:L:52:ILE:HG22	4:L:70:ALA:HB2	2.00	0.44
2:B:335:LEU:HB2	2:B:338:LEU:HB2	2.01	0.43
3:C:266:ARG:NE	3:C:380:GLN:HE21	2.18	0.42
6:B:402:Y01:CBH	6:B:402:Y01:HBF	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:404:Y01:HAC1	6:A:404:Y01:HAU2	2.02	0.41
2:B:127:GLU:OE2	5:H:118:ARG:NE	2.54	0.41
2:B:125:ILE:O	5:H:118:ARG:NH1	2.50	0.41
3:C:361:LYS:HA	3:C:364:ARG:HG2	2.01	0.41
1:A:18:TRP:HA	1:A:21:ILE:HG22	2.02	0.41
6:A:402:Y01:HAK1	6:A:402:Y01:HAE1	2.03	0.41
6:A:403:Y01:HAE1	6:A:403:Y01:HAK1	2.02	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/364 (66%)	226 (95%)	13 (5%)	0	100	100
2	B	275/301 (91%)	265 (96%)	10 (4%)	0	100	100
3	C	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
4	L	104/214 (49%)	97 (93%)	7 (7%)	0	100	100
5	H	116/232 (50%)	109 (94%)	7 (6%)	0	100	100
All	All	852/1231 (69%)	809 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/328 (66%)	216 (100%)	0	100	100
2	B	230/248 (93%)	226 (98%)	4 (2%)	60	80
3	C	98/98 (100%)	97 (99%)	1 (1%)	76	87
4	L	92/189 (49%)	91 (99%)	1 (1%)	73	86
5	H	100/200 (50%)	98 (98%)	2 (2%)	55	78
All	All	736/1063 (69%)	728 (99%)	8 (1%)	74	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	62	LEU
2	B	112	ASP
2	B	180	PHE
2	B	283	LEU
3	C	300	ARG
4	L	115	TYR
5	H	49	THR
5	H	125	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
2	B	95	HIS
2	B	299	GLN
4	L	25	GLN
4	L	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	Y01	A	403	-	38,38,38	4.63	16 (42%)	57,57,57	2.52	23 (40%)
6	Y01	B	402	-	38,38,38	4.75	18 (47%)	57,57,57	1.76	14 (24%)
6	Y01	A	405	-	38,38,38	4.73	18 (47%)	57,57,57	2.10	17 (29%)
7	AJP	A	406	-	83,83,95	7.31	46 (55%)	125,131,149	2.02	40 (32%)
6	Y01	A	404	-	38,38,38	4.77	17 (44%)	57,57,57	1.93	17 (29%)
6	Y01	A	402	-	38,38,38	4.63	16 (42%)	57,57,57	2.21	22 (38%)
6	Y01	A	401	-	38,38,38	4.73	18 (47%)	57,57,57	1.94	17 (29%)
7	AJP	B	401	-	49,49,95	9.39	35 (71%)	74,80,149	2.40	29 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	Y01	A	403	-	1/1/12/13	8/19/77/77	0/4/4/4
6	Y01	B	402	-	1/1/12/13	12/19/77/77	0/4/4/4
6	Y01	A	405	-	1/1/12/13	10/19/77/77	0/4/4/4
7	AJP	A	406	-	29/29/33/38	14/22/194/220	0/10/10/11
6	Y01	A	404	-	1/1/12/13	7/19/77/77	0/4/4/4
6	Y01	A	402	-	1/1/12/13	17/19/77/77	0/4/4/4
6	Y01	A	401	-	1/1/12/13	9/19/77/77	0/4/4/4
7	AJP	B	401	-	16/16/19/38	3/6/121/220	0/7/7/11

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	AJP	C07-C08	27.50	2.01	1.53
7	A	406	AJP	C07-C08	27.36	2.00	1.53
7	A	406	AJP	O09-C08	-26.00	1.00	1.43
7	B	401	AJP	O09-C08	-25.45	1.01	1.43
7	B	401	AJP	O84-C05	-24.07	1.05	1.42
7	A	406	AJP	O84-C05	-23.88	1.05	1.42
7	B	401	AJP	C04-C05	-18.70	1.22	1.52
7	A	406	AJP	C04-C05	-18.54	1.22	1.52
7	B	401	AJP	O09-C05	17.26	1.80	1.42
7	A	406	AJP	O09-C05	17.02	1.79	1.42
7	B	401	AJP	C12-C07	-16.76	1.22	1.56
6	A	402	Y01	CAI-CAZ	16.60	1.69	1.33
6	A	404	Y01	CAI-CAZ	16.53	1.69	1.33
6	A	401	Y01	CAI-CAZ	16.50	1.69	1.33
7	A	406	AJP	C12-C07	-16.45	1.22	1.56
6	A	403	Y01	CAI-CAZ	16.34	1.69	1.33
6	A	405	Y01	CAI-CAZ	16.29	1.68	1.33
6	B	402	Y01	CAI-CAZ	16.29	1.68	1.33
7	A	406	AJP	C03-C02	-15.30	1.10	1.52
7	B	401	AJP	C03-C02	-14.99	1.11	1.52
7	B	401	AJP	C01-C02	14.16	1.97	1.52
7	A	406	AJP	C01-C02	13.62	1.96	1.52
7	A	406	AJP	C12-C11	12.86	1.82	1.56
7	B	401	AJP	C12-C11	12.68	1.81	1.56
7	A	406	AJP	C16-C15	12.64	1.77	1.53
7	A	406	AJP	C85-C02	-12.62	1.20	1.51
7	B	401	AJP	C85-C02	-12.41	1.20	1.51
6	A	405	Y01	CBH-CBF	11.91	1.76	1.56
7	B	401	AJP	C16-C15	11.77	1.76	1.53
6	B	402	Y01	CBH-CBF	11.69	1.75	1.56
6	A	401	Y01	CBH-CBF	11.57	1.75	1.56
6	A	404	Y01	CBH-CBF	11.52	1.75	1.56
6	A	402	Y01	CBH-CBF	10.12	1.73	1.56
6	A	403	Y01	CBH-CBF	10.10	1.73	1.56
7	B	401	AJP	C11-C10	9.68	1.72	1.53
7	A	406	AJP	C10-C08	-9.55	1.31	1.52
6	A	404	Y01	CBI-CBE	9.53	1.73	1.55
6	A	403	Y01	CBB-CBE	-9.44	1.37	1.54
7	B	401	AJP	C10-C08	-9.34	1.32	1.52
7	A	406	AJP	C11-C10	9.07	1.71	1.53
6	B	402	Y01	CBI-CBE	9.07	1.72	1.55
6	A	404	Y01	CBB-CBE	-9.06	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	402	Y01	CBB-CBE	-8.98	1.38	1.54
6	A	402	Y01	CBB-CBE	-8.63	1.39	1.54
6	A	402	Y01	CBI-CBE	8.53	1.71	1.55
6	A	401	Y01	CBI-CBE	8.52	1.71	1.55
6	A	401	Y01	CBB-CBE	-8.41	1.39	1.54
6	A	405	Y01	CBI-CBE	8.33	1.70	1.55
6	A	403	Y01	CBI-CBE	8.32	1.70	1.55
6	A	405	Y01	CBB-CBE	-8.23	1.40	1.54
6	A	405	Y01	CAU-CBI	-7.91	1.39	1.54
6	A	401	Y01	CAK-CBD	7.76	1.66	1.53
6	B	402	Y01	CAK-CBD	7.69	1.66	1.53
7	A	406	AJP	C14-C15	7.66	1.66	1.53
6	A	404	Y01	CAK-CBD	7.65	1.66	1.53
6	A	402	Y01	CAK-CBD	7.61	1.66	1.53
6	A	405	Y01	CAK-CBD	7.43	1.65	1.53
6	A	403	Y01	CAK-CBD	7.41	1.65	1.53
6	A	402	Y01	CAU-CBI	-7.35	1.40	1.54
6	A	401	Y01	CAU-CBI	-7.31	1.41	1.54
7	B	401	AJP	C14-C15	7.20	1.65	1.53
6	B	402	Y01	CAU-CBI	-7.17	1.41	1.54
6	A	404	Y01	CAU-CBI	-7.16	1.41	1.54
6	A	403	Y01	CAU-CBI	-6.93	1.41	1.54
7	A	406	AJP	C16-C11	-6.45	1.45	1.54
6	A	402	Y01	CAP-CBE	6.33	1.67	1.54
6	A	401	Y01	CAP-CBE	6.33	1.67	1.54
7	B	401	AJP	C16-C11	-6.31	1.45	1.54
6	A	405	Y01	CAP-CBE	6.20	1.67	1.54
6	A	404	Y01	CAP-CBE	6.12	1.67	1.54
6	A	403	Y01	CAP-CBE	6.10	1.67	1.54
6	B	402	Y01	CAP-CBE	6.07	1.67	1.54
7	B	401	AJP	C13-C12	-5.66	1.44	1.54
7	A	406	AJP	C13-C12	-5.27	1.44	1.54
6	A	401	Y01	CAU-CAS	5.16	1.64	1.53
7	A	406	AJP	O84-C85	5.00	1.50	1.43
6	A	402	Y01	CAU-CAS	4.97	1.64	1.53
6	B	402	Y01	CAU-CAS	4.95	1.63	1.53
6	A	403	Y01	CAQ-CBG	4.85	1.64	1.54
6	A	405	Y01	CAU-CAS	4.78	1.63	1.53
7	B	401	AJP	O84-C85	4.74	1.50	1.43
6	A	405	Y01	CAQ-CBG	4.73	1.64	1.54
7	B	401	AJP	C17-C16	-4.70	1.44	1.53
7	A	406	AJP	C20-C15	-4.69	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	AJP	C20-C15	-4.60	1.47	1.56
6	A	404	Y01	CAU-CAS	4.60	1.63	1.53
7	B	401	AJP	C24-C23	4.56	1.60	1.52
6	A	401	Y01	CAQ-CBG	4.43	1.63	1.54
7	A	406	AJP	C24-C23	4.40	1.60	1.52
7	B	401	AJP	C18-C19	4.40	1.64	1.53
7	A	406	AJP	C18-C19	4.34	1.63	1.53
6	B	402	Y01	CAQ-CBG	4.33	1.63	1.54
6	A	404	Y01	CAQ-CBG	4.31	1.63	1.54
6	A	403	Y01	CAU-CAS	4.28	1.62	1.53
7	A	406	AJP	O25-C23	-4.12	1.37	1.44
6	A	405	Y01	OAW-CAY	4.10	1.45	1.34
6	A	403	Y01	OAW-CAY	4.08	1.45	1.34
6	A	402	Y01	OAW-CAY	4.02	1.45	1.34
6	B	402	Y01	OAW-CAY	3.99	1.45	1.34
6	A	401	Y01	OAW-CAY	3.99	1.45	1.34
7	A	406	AJP	O50-C49	3.93	1.50	1.43
6	A	402	Y01	CAO-CBB	3.86	1.64	1.54
6	A	402	Y01	CAQ-CBG	3.84	1.62	1.54
6	A	404	Y01	OAW-CAY	3.77	1.44	1.34
6	B	402	Y01	CAO-CBB	3.67	1.63	1.54
7	B	401	AJP	C07-C06	-3.64	1.42	1.54
6	A	402	Y01	CAC-CBB	3.64	1.62	1.53
6	A	401	Y01	CAO-CBB	3.59	1.63	1.54
6	A	404	Y01	CAE-CBI	3.57	1.60	1.54
6	A	403	Y01	CAE-CBI	3.57	1.60	1.54
6	A	405	Y01	CAO-CBB	3.55	1.63	1.54
6	A	405	Y01	CAE-CBI	3.51	1.60	1.54
6	A	403	Y01	CAQ-CAP	3.51	1.63	1.54
7	A	406	AJP	O40-C35	3.45	1.50	1.41
7	B	401	AJP	C05-C06	3.40	1.60	1.53
6	A	403	Y01	CAC-CBB	3.40	1.61	1.53
7	A	406	AJP	C07-C06	-3.39	1.43	1.54
7	A	406	AJP	C17-C16	-3.37	1.47	1.53
6	B	402	Y01	CAE-CBI	3.34	1.60	1.54
6	A	404	Y01	CAO-CBB	3.34	1.63	1.54
7	B	401	AJP	O25-C23	-3.33	1.39	1.44
6	A	405	Y01	CAC-CBB	3.33	1.61	1.53
6	A	402	Y01	CAE-CBI	3.31	1.60	1.54
6	A	403	Y01	CAO-CBB	3.30	1.62	1.54
7	A	406	AJP	C05-C06	3.28	1.59	1.53
6	A	405	Y01	CAQ-CAP	3.28	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	AJP	C22-C23	3.27	1.57	1.52
6	A	401	Y01	CAC-CBB	3.26	1.61	1.53
6	A	401	Y01	CAE-CBI	3.25	1.60	1.54
7	A	406	AJP	C83-C06	3.25	1.60	1.53
7	A	406	AJP	C21-C22	3.22	1.58	1.53
7	A	406	AJP	C22-C23	3.18	1.57	1.52
6	B	402	Y01	CAC-CBB	3.16	1.60	1.53
6	A	404	Y01	CAC-CBB	3.13	1.60	1.53
6	A	401	Y01	CAQ-CAP	2.94	1.62	1.54
6	A	404	Y01	CAQ-CAP	2.94	1.62	1.54
6	B	402	Y01	CAQ-CAP	2.93	1.62	1.54
6	A	403	Y01	CBH-CAZ	-2.93	1.47	1.52
7	B	401	AJP	C83-C06	2.92	1.59	1.53
6	A	402	Y01	CAQ-CAP	2.88	1.61	1.54
7	A	406	AJP	O64-C57	2.86	1.49	1.43
7	A	406	AJP	O50-C45	2.84	1.47	1.41
7	A	406	AJP	C18-C17	2.83	1.59	1.52
7	A	406	AJP	O60-C55	2.78	1.48	1.41
6	A	404	Y01	CBH-CAZ	-2.69	1.47	1.52
7	A	406	AJP	O44-C37	2.66	1.50	1.43
7	B	401	AJP	C18-C17	2.57	1.59	1.52
6	B	402	Y01	CBH-CAZ	-2.56	1.47	1.52
6	A	402	Y01	CBH-CAZ	-2.56	1.47	1.52
7	A	406	AJP	C48-C47	-2.51	1.48	1.52
6	B	402	Y01	CBD-CBG	2.44	1.58	1.53
7	B	401	AJP	C21-C22	2.43	1.56	1.53
6	A	405	Y01	CBD-CBG	2.42	1.58	1.53
7	B	401	AJP	O31-C26	2.39	1.47	1.41
7	A	406	AJP	O60-C59	2.33	1.50	1.44
7	B	401	AJP	C20-C19	2.33	1.59	1.55
7	B	401	AJP	C04-C03	-2.32	1.48	1.53
6	A	405	Y01	CAV-CAZ	2.30	1.56	1.51
6	A	404	Y01	CBD-CBG	2.30	1.58	1.53
7	A	406	AJP	C81-C12	2.26	1.58	1.54
7	A	406	AJP	C21-C20	2.25	1.57	1.54
7	A	406	AJP	C04-C03	-2.25	1.48	1.53
6	A	401	Y01	CBH-CAZ	-2.25	1.48	1.52
7	A	406	AJP	C28-C29	-2.19	1.46	1.52
7	B	401	AJP	C29-C28	-2.18	1.46	1.52
6	A	405	Y01	CBH-CAZ	-2.17	1.48	1.52
7	A	406	AJP	C13-C14	2.16	1.58	1.53
7	A	406	AJP	O34-C29	2.16	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	401	Y01	CBD-CBG	2.15	1.57	1.53
6	B	402	Y01	CAD-CBH	2.14	1.58	1.54
7	B	401	AJP	C81-C12	2.13	1.58	1.54
7	A	406	AJP	O79-C22	-2.10	1.38	1.43
7	B	401	AJP	O34-C29	2.10	1.47	1.43
7	A	406	AJP	O31-C26	2.09	1.47	1.41
6	A	404	Y01	CAV-CAZ	2.08	1.56	1.51
6	B	402	Y01	CAM-CAY	2.07	1.56	1.50
7	A	406	AJP	C20-C19	2.06	1.58	1.55
6	A	402	Y01	CBD-CBF	-2.05	1.49	1.53
6	A	405	Y01	CAM-CAY	2.05	1.56	1.50
6	A	401	Y01	CAM-CAY	2.03	1.56	1.50
7	B	401	AJP	O79-C22	-2.02	1.39	1.43
6	A	401	Y01	CAV-CAZ	2.02	1.56	1.51
7	A	406	AJP	O54-C36	2.02	1.49	1.43
6	A	403	Y01	CAM-CAY	2.02	1.56	1.50

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	403	Y01	CBH-CAZ-CAI	-6.71	112.63	122.90
7	B	401	AJP	C24-C23-C22	6.69	118.09	111.00
7	A	406	AJP	C24-C23-C22	6.20	117.57	111.00
7	B	401	AJP	C03-C02-C85	5.59	116.33	108.56
7	A	406	AJP	C21-C20-C15	5.52	118.33	110.08
7	B	401	AJP	O09-C08-C10	5.46	121.40	110.17
6	A	403	Y01	CAP-CBE-CBB	5.25	120.27	112.15
6	A	404	Y01	CBF-CBD-CBG	5.15	115.99	109.09
6	A	402	Y01	CBH-CAZ-CAI	-5.11	115.09	122.90
6	A	403	Y01	CAQ-CBG-CBD	5.09	127.47	119.08
6	B	402	Y01	CBF-CBD-CBG	4.88	115.62	109.09
6	A	405	Y01	CAP-CBE-CBB	4.87	119.69	112.15
6	A	403	Y01	CAU-CBI-CBG	4.85	114.80	107.27
6	A	405	Y01	CBF-CBD-CBG	4.69	115.37	109.09
6	A	402	Y01	CAP-CBE-CBB	4.65	119.35	112.15
6	A	403	Y01	CBI-CBE-CBB	-4.64	112.22	119.49
7	A	406	AJP	C13-C12-C07	4.64	122.87	115.46
7	B	401	AJP	C12-C07-C06	4.63	136.31	120.56
7	B	401	AJP	C26-O25-C23	4.60	122.44	115.33
7	A	406	AJP	C20-C15-C16	-4.57	107.62	112.42
6	A	405	Y01	CAK-CAI-CAZ	-4.57	116.63	125.06
6	A	404	Y01	CAK-CAI-CAZ	-4.57	116.63	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	401	AJP	C85-O84-C05	4.52	122.29	113.72
6	B	402	Y01	OAW-CAY-CAM	4.49	121.17	111.50
6	A	401	Y01	CAK-CAI-CAZ	-4.45	116.85	125.06
6	B	402	Y01	CAK-CAI-CAZ	-4.37	116.99	125.06
7	A	406	AJP	C35-C36-C37	-4.30	102.16	110.75
7	A	406	AJP	C14-C15-C16	4.25	117.88	111.75
6	A	403	Y01	CAV-CAZ-CAI	-4.24	114.49	120.61
7	A	406	AJP	C03-C02-C85	4.24	114.45	108.56
6	A	402	Y01	CAV-CAZ-CAI	-4.23	114.52	120.61
7	A	406	AJP	O09-C08-C10	4.21	118.83	110.17
6	A	403	Y01	CAR-CBC-CAV	4.19	117.23	110.99
7	A	406	AJP	O25-C23-C24	-4.15	101.60	109.62
6	A	403	Y01	CAK-CAI-CAZ	-4.12	117.45	125.06
7	A	406	AJP	C12-C07-C06	4.11	134.55	120.56
6	A	403	Y01	CAT-CAR-CBC	4.06	117.25	110.33
7	B	401	AJP	C13-C12-C07	4.04	121.92	115.46
7	B	401	AJP	O84-C85-C02	4.03	117.99	112.18
6	A	401	Y01	CBH-CAZ-CAI	-4.02	116.75	122.90
6	A	402	Y01	CAK-CAI-CAZ	-4.01	117.66	125.06
6	A	401	Y01	CAP-CBE-CBB	3.96	118.28	112.15
6	A	405	Y01	CBH-CAZ-CAI	-3.94	116.88	122.90
6	A	402	Y01	CAU-CBI-CBG	3.89	113.31	107.27
7	B	401	AJP	C81-C12-C11	-3.87	102.21	111.63
6	A	405	Y01	CBF-CBH-CAZ	3.86	115.70	109.65
6	A	401	Y01	CAU-CBI-CBE	3.83	122.31	116.57
6	A	405	Y01	CAP-CBE-CBI	-3.81	99.25	103.84
6	A	402	Y01	CAR-CBC-CAV	3.77	116.61	110.99
6	A	404	Y01	CBH-CAZ-CAI	-3.77	117.13	122.90
6	A	405	Y01	OAW-CAY-CAM	3.69	119.46	111.50
6	A	402	Y01	OAW-CAY-CAM	3.69	119.45	111.50
7	B	401	AJP	C20-C15-C16	-3.65	108.58	112.42
6	A	401	Y01	CBF-CBD-CBG	3.63	113.95	109.09
7	B	401	AJP	C03-C04-C05	3.62	118.19	111.93
6	A	404	Y01	OAW-CAY-CAM	3.62	119.30	111.50
7	A	406	AJP	O84-C05-C04	3.60	114.12	110.77
7	A	406	AJP	C49-C48-C47	3.58	114.07	109.67
7	B	401	AJP	C04-C03-C02	3.51	119.21	111.81
6	A	401	Y01	OAW-CAY-CAM	3.49	119.03	111.50
6	A	403	Y01	CAD-CBH-CBF	-3.46	107.56	111.68
6	B	402	Y01	CAU-CBI-CBE	3.45	121.73	116.57
6	A	405	Y01	CAQ-CBG-CBD	3.39	124.67	119.08
6	A	403	Y01	OAW-CAY-CAM	3.35	118.72	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	401	AJP	C06-C07-C08	-3.35	98.24	104.34
7	A	406	AJP	C21-C20-C19	-3.29	103.42	107.14
6	A	404	Y01	CAD-CBH-CAZ	-3.29	103.01	108.34
7	A	406	AJP	O34-C35-C36	3.27	115.74	109.10
7	B	401	AJP	O25-C26-C27	3.27	116.58	108.10
6	A	401	Y01	CBI-CBE-CBB	-3.27	114.37	119.49
7	A	406	AJP	O44-C37-C38	3.26	115.94	107.28
6	A	404	Y01	CBI-CBG-CBD	3.25	119.19	114.38
6	A	403	Y01	CAJ-CAO-CBB	-3.23	105.74	115.03
7	A	406	AJP	C81-C12-C11	-3.21	103.81	111.63
6	A	405	Y01	CAK-CBD-CBF	3.15	113.54	109.71
6	A	403	Y01	CAU-CAS-CBF	-3.13	107.69	113.11
6	A	402	Y01	CAD-CBH-CBF	-3.11	107.97	111.68
7	B	401	AJP	C14-C15-C16	3.11	116.23	111.75
7	A	406	AJP	O25-C26-O31	-3.09	102.05	110.67
6	A	404	Y01	CAU-CBI-CBE	3.07	121.17	116.57
6	A	403	Y01	CAP-CBE-CBI	-3.07	100.15	103.84
6	A	402	Y01	CAU-CBI-CBE	3.06	121.15	116.57
6	A	401	Y01	CAU-CBI-CBG	3.05	112.00	107.27
6	A	401	Y01	CBI-CBG-CBD	3.04	118.88	114.38
6	A	402	Y01	CAT-CAR-CBC	3.04	115.51	110.33
6	A	405	Y01	CAU-CBI-CBG	3.04	111.98	107.27
7	A	406	AJP	C03-C04-C05	3.03	117.18	111.93
6	A	401	Y01	OAW-CBC-CAV	3.03	114.31	108.12
6	A	402	Y01	CBG-CBI-CBE	-3.01	96.51	100.07
6	A	405	Y01	CBI-CBE-CBB	-2.99	114.80	119.49
6	A	401	Y01	CAE-CBI-CBE	-2.93	106.25	111.71
6	A	403	Y01	CBG-CBI-CBE	-2.91	96.62	100.07
7	A	406	AJP	C80-C20-C15	-2.91	107.17	111.18
7	A	406	AJP	C81-C12-C13	-2.91	106.00	110.59
6	B	402	Y01	CBI-CBG-CBD	2.87	118.64	114.38
6	A	402	Y01	CAC-CBB-CAO	2.87	114.85	110.36
6	A	401	Y01	CAP-CBE-CBI	-2.86	100.40	103.84
6	A	405	Y01	CAV-CAZ-CAI	-2.82	116.55	120.61
6	A	403	Y01	CAE-CBI-CAU	-2.81	106.15	110.59
6	B	402	Y01	CBH-CAZ-CAI	-2.77	118.66	122.90
6	A	403	Y01	CAD-CBH-CAZ	2.77	112.83	108.34
6	A	402	Y01	CBI-CBG-CBD	2.75	118.46	114.38
6	A	404	Y01	CAR-CBC-CAV	2.75	115.09	110.99
6	B	402	Y01	CAK-CBD-CBF	2.73	113.02	109.71
7	A	406	AJP	O77-C28-C27	-2.73	104.05	110.35
7	A	406	AJP	C17-C18-C19	2.71	117.28	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	Y01	CAE-CBI-CBE	-2.69	106.70	111.71
7	A	406	AJP	O09-C08-C07	2.67	110.48	104.06
6	A	402	Y01	CAC-CBB-CBE	-2.67	108.84	112.92
6	A	403	Y01	CAU-CBI-CBE	2.66	120.56	116.57
6	A	402	Y01	CAK-CBD-CBF	2.66	112.94	109.71
7	B	401	AJP	C11-C12-C07	-2.66	95.65	100.19
7	B	401	AJP	C81-C12-C13	-2.65	106.41	110.59
7	B	401	AJP	C04-C05-C06	2.63	121.10	115.69
7	A	406	AJP	C06-C07-C08	-2.56	99.68	104.34
7	A	406	AJP	O54-C36-C35	2.55	114.99	108.61
7	B	401	AJP	O84-C05-C04	2.55	113.14	110.77
6	A	401	Y01	CAE-CBI-CAU	-2.54	106.58	110.59
7	B	401	AJP	O09-C08-C07	2.53	110.13	104.06
6	A	404	Y01	CAK-CBD-CBF	2.52	112.77	109.71
6	B	402	Y01	CAT-CAR-CBC	2.50	114.60	110.33
6	A	404	Y01	CBD-CAK-CAI	-2.50	109.14	112.73
7	A	406	AJP	C26-O25-C23	2.50	119.19	115.33
6	A	402	Y01	CBI-CBE-CBB	-2.49	115.58	119.49
6	B	402	Y01	CAE-CBI-CAU	-2.48	106.67	110.59
6	A	402	Y01	CAE-CBI-CAU	-2.48	106.67	110.59
7	A	406	AJP	O44-C37-C36	2.47	113.77	107.48
6	A	405	Y01	CAO-CBB-CBE	2.47	115.39	110.28
7	B	401	AJP	O84-C05-O09	-2.47	102.90	109.78
6	A	403	Y01	CBF-CBD-CBG	2.42	112.33	109.09
7	A	406	AJP	C12-C07-C08	-2.40	102.28	104.88
6	A	404	Y01	CAQ-CBG-CBD	2.39	123.02	119.08
7	B	401	AJP	C13-C12-C11	2.38	112.94	108.19
6	A	405	Y01	CAU-CBI-CBE	2.37	120.12	116.57
6	A	402	Y01	CAV-CAZ-CBH	-2.36	113.28	116.42
6	A	403	Y01	CAO-CBB-CBE	2.36	115.16	110.28
7	A	406	AJP	C83-C06-C07	2.36	119.73	114.50
6	B	402	Y01	CAE-CBI-CBE	-2.34	107.35	111.71
7	B	401	AJP	O78-C27-C28	-2.34	104.94	110.35
6	A	405	Y01	CBI-CBG-CBD	2.31	117.80	114.38
6	B	402	Y01	CAQ-CBG-CBD	2.30	122.86	119.08
6	A	403	Y01	CBC-CAV-CAZ	2.29	115.08	111.52
7	B	401	AJP	C01-C02-C85	-2.28	107.17	111.18
6	A	404	Y01	CAE-CBI-CBE	-2.26	107.50	111.71
6	A	401	Y01	CAK-CBD-CBF	2.26	112.45	109.71
6	A	405	Y01	CAE-CBI-CAU	-2.26	107.02	110.59
6	A	404	Y01	CAE-CBI-CAU	-2.26	107.03	110.59
7	B	401	AJP	C83-C06-C05	2.25	119.03	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	402	Y01	OAH-CAX-CAL	2.25	121.26	114.03
6	A	403	Y01	CAC-CBB-CBE	-2.21	109.53	112.92
6	A	403	Y01	CAT-CBH-CBF	2.21	111.81	108.73
7	A	406	AJP	O31-C30-C29	2.21	114.40	109.75
7	B	401	AJP	C05-C06-C07	-2.20	99.79	103.37
6	A	402	Y01	CAD-CBH-CAZ	2.20	111.91	108.34
6	A	401	Y01	CAO-CBB-CBE	2.19	114.82	110.28
6	A	402	Y01	CAO-CBB-CBE	2.19	114.82	110.28
7	A	406	AJP	O60-C59-C58	2.17	113.63	109.69
7	A	406	AJP	O40-C35-C36	2.17	113.80	109.51
6	B	402	Y01	CAE-CBI-CBG	-2.16	107.68	111.71
6	A	404	Y01	OAH-CAX-CAL	2.15	120.94	114.03
7	A	406	AJP	C17-C16-C11	2.15	115.45	112.32
6	B	402	Y01	CAU-CBI-CBG	2.14	110.59	107.27
7	A	406	AJP	C14-C13-C12	2.14	116.45	112.78
6	B	402	Y01	CAP-CBE-CBI	-2.13	101.28	103.84
6	A	404	Y01	CAT-CAR-CBC	2.12	113.95	110.33
7	B	401	AJP	C18-C19-C20	2.11	116.09	112.31
7	A	406	AJP	C35-O40-C39	2.11	117.82	113.69
6	A	402	Y01	OAW-CBC-CAR	2.10	113.39	108.33
7	A	406	AJP	C85-O84-C05	2.10	117.69	113.72
7	A	406	AJP	O54-C55-C56	2.06	113.45	108.10
7	A	406	AJP	O34-C29-C30	2.06	115.10	109.45
7	A	406	AJP	C18-C19-C20	2.05	115.99	112.31
7	B	401	AJP	C14-C13-C12	2.05	116.29	112.78
7	B	401	AJP	C17-C16-C15	-2.04	107.96	110.49
7	A	406	AJP	O84-C05-O09	-2.03	104.11	109.78
6	A	401	Y01	CBD-CAK-CAI	-2.03	109.82	112.73
6	A	404	Y01	CBC-CAV-CAZ	2.02	114.66	111.52
6	A	404	Y01	CAU-CBI-CBG	2.02	110.41	107.27
6	A	401	Y01	CAQ-CBG-CBD	2.02	122.40	119.08

All (51) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	401	Y01	CBD
6	A	402	Y01	CBD
6	A	403	Y01	CBD
6	A	404	Y01	CBD
6	A	405	Y01	CBD
6	B	402	Y01	CBD
7	A	406	AJP	C38

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Mol	Chain	Res	Type	Atom
7	A	406	AJP	C47
7	A	406	AJP	C02
7	A	406	AJP	C11
7	A	406	AJP	C26
7	A	406	AJP	C16
7	A	406	AJP	C46
7	A	406	AJP	C12
7	A	406	AJP	C56
7	A	406	AJP	C15
7	A	406	AJP	C36
7	A	406	AJP	C28
7	A	406	AJP	C37
7	A	406	AJP	C10
7	A	406	AJP	C30
7	A	406	AJP	C22
7	A	406	AJP	C27
7	A	406	AJP	C20
7	A	406	AJP	C35
7	A	406	AJP	C23
7	A	406	AJP	C55
7	A	406	AJP	C19
7	A	406	AJP	C39
7	A	406	AJP	C48
7	A	406	AJP	C59
7	A	406	AJP	C07
7	A	406	AJP	C05
7	A	406	AJP	C57
7	A	406	AJP	C45
7	B	401	AJP	C27
7	B	401	AJP	C20
7	B	401	AJP	C28
7	B	401	AJP	C12
7	B	401	AJP	C23
7	B	401	AJP	C26
7	B	401	AJP	C19
7	B	401	AJP	C10
7	B	401	AJP	C30
7	B	401	AJP	C02
7	B	401	AJP	C07
7	B	401	AJP	C11
7	B	401	AJP	C05
7	B	401	AJP	C22

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Mol	Chain	Res	Type	Atom
7	B	401	AJP	C15
7	B	401	AJP	C16

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	Y01	CAV-CBC-OAW-CAY
6	A	402	Y01	CAR-CBC-OAW-CAY
6	A	403	Y01	CAR-CBC-OAW-CAY
6	A	404	Y01	CAM-CAY-OAW-CBC
6	A	405	Y01	CAO-CBB-CBE-CAP
6	A	405	Y01	CAC-CBB-CBE-CBI
6	A	405	Y01	CAR-CBC-OAW-CAY
6	B	402	Y01	CAV-CBC-OAW-CAY
6	B	402	Y01	OAG-CAY-OAW-CBC
6	B	402	Y01	CAX-CAL-CAM-CAY
7	B	401	AJP	C27-C26-O25-C23
7	A	406	AJP	O31-C26-O25-C23
7	A	406	AJP	C27-C26-O25-C23
6	A	405	Y01	CAC-CBB-CBE-CAP
6	A	401	Y01	CAC-CBB-CBE-CBI
6	A	405	Y01	CAO-CBB-CBE-CBI
6	B	402	Y01	CAM-CAY-OAW-CBC
6	A	402	Y01	CAJ-CAO-CBB-CAC
6	A	401	Y01	CAC-CBB-CBE-CAP
6	A	401	Y01	CAO-CBB-CBE-CBI
6	A	404	Y01	OAG-CAY-OAW-CBC
6	A	401	Y01	CAO-CBB-CBE-CAP
6	A	402	Y01	CAM-CAY-OAW-CBC
6	A	405	Y01	CAM-CAY-OAW-CBC
7	A	406	AJP	C30-C29-O34-C35
6	B	402	Y01	CAJ-CAO-CBB-CAC
6	A	402	Y01	CAJ-CAO-CBB-CBE
6	B	402	Y01	CAJ-CAO-CBB-CBE
6	A	405	Y01	OAG-CAY-OAW-CBC
6	A	402	Y01	CAO-CBB-CBE-CBI
6	A	402	Y01	OAG-CAY-OAW-CBC
6	A	402	Y01	CAO-CAJ-CAN-CBA
6	B	402	Y01	CAO-CAJ-CAN-CBA
7	A	406	AJP	C37-C36-O54-C55
6	A	401	Y01	CAO-CAJ-CAN-CBA
6	B	402	Y01	CAN-CAJ-CAO-CBB

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Mol	Chain	Res	Type	Atoms
6	A	403	Y01	CAM-CAY-OAW-CBC
6	A	402	Y01	CAC-CBB-CBE-CAP
6	A	402	Y01	CAC-CBB-CBE-CBI
7	A	406	AJP	C38-C37-O44-C45
6	A	404	Y01	CAN-CAJ-CAO-CBB
6	A	405	Y01	CAO-CAJ-CAN-CBA
6	A	403	Y01	OAG-CAY-OAW-CBC
6	A	402	Y01	CAJ-CAN-CBA-CAB
7	A	406	AJP	C38-C39-C41-O42
6	A	402	Y01	CAX-CAL-CAM-CAY
7	A	406	AJP	C28-C29-O34-C35
6	A	402	Y01	CAJ-CAN-CBA-CAA
6	A	404	Y01	CAO-CAJ-CAN-CBA
7	B	401	AJP	O31-C30-C32-O33
7	B	401	AJP	O31-C26-O25-C23
7	A	406	AJP	O31-C30-C32-O33
7	A	406	AJP	C36-C37-O44-C45
6	A	404	Y01	CAJ-CAN-CBA-CAA
7	A	406	AJP	C56-C55-O54-C36
6	A	403	Y01	CAJ-CAN-CBA-CAB
6	A	401	Y01	CAM-CAY-OAW-CBC
6	A	401	Y01	OAG-CAY-OAW-CBC
6	A	404	Y01	CAJ-CAN-CBA-CAB
6	A	403	Y01	CAJ-CAN-CBA-CAA
6	A	401	Y01	CAN-CAJ-CAO-CBB
7	A	406	AJP	O60-C55-O54-C36
6	A	403	Y01	CAO-CAJ-CAN-CBA
6	A	405	Y01	CAM-CAL-CAX-OAF
7	A	406	AJP	O40-C35-O34-C29
7	A	406	AJP	O40-C39-C41-O42
6	A	405	Y01	CAM-CAL-CAX-OAH
6	A	402	Y01	CAM-CAL-CAX-OAF
6	A	402	Y01	CAO-CBB-CBE-CAP
6	A	403	Y01	CAM-CAL-CAX-OAF
6	B	402	Y01	CAM-CAL-CAX-OAH
6	B	402	Y01	CAM-CAL-CAX-OAF
6	A	403	Y01	CAM-CAL-CAX-OAH
6	A	402	Y01	CAM-CAL-CAX-OAH
7	A	406	AJP	C35-C36-O54-C55
6	A	402	Y01	CAL-CAM-CAY-OAW
6	A	402	Y01	CAN-CAJ-CAO-CBB
6	B	402	Y01	CAR-CBC-OAW-CAY

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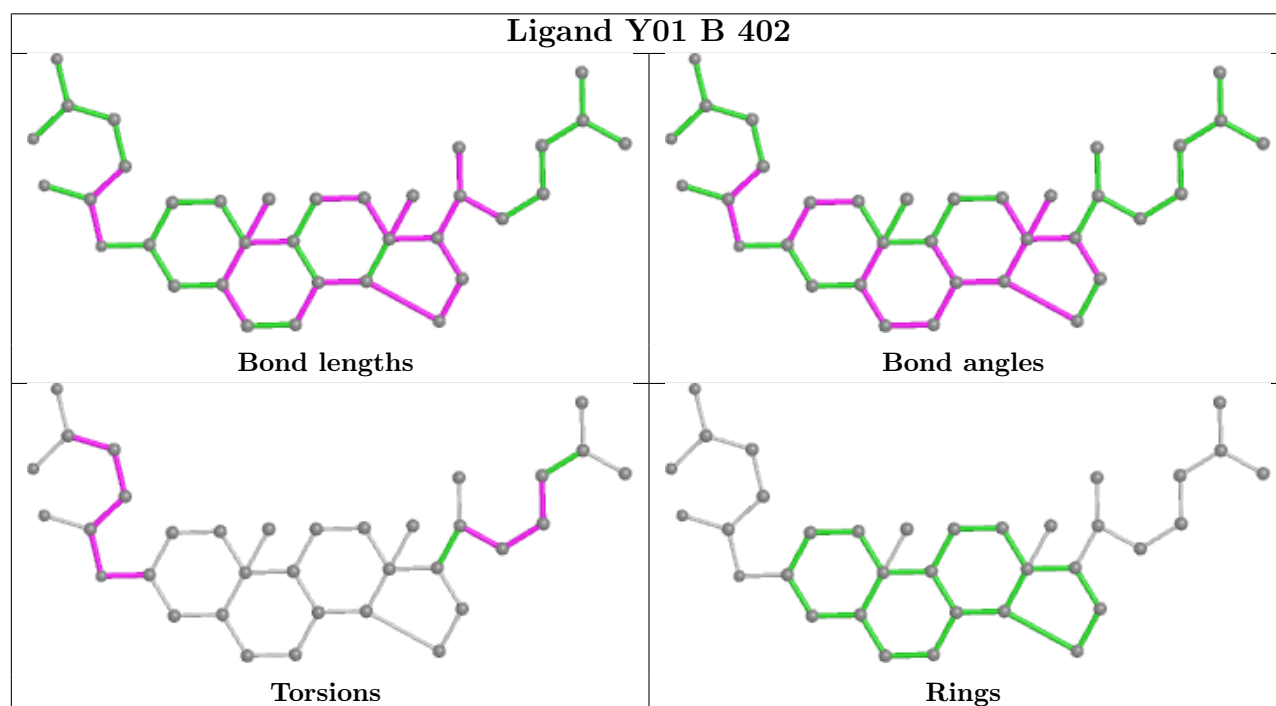
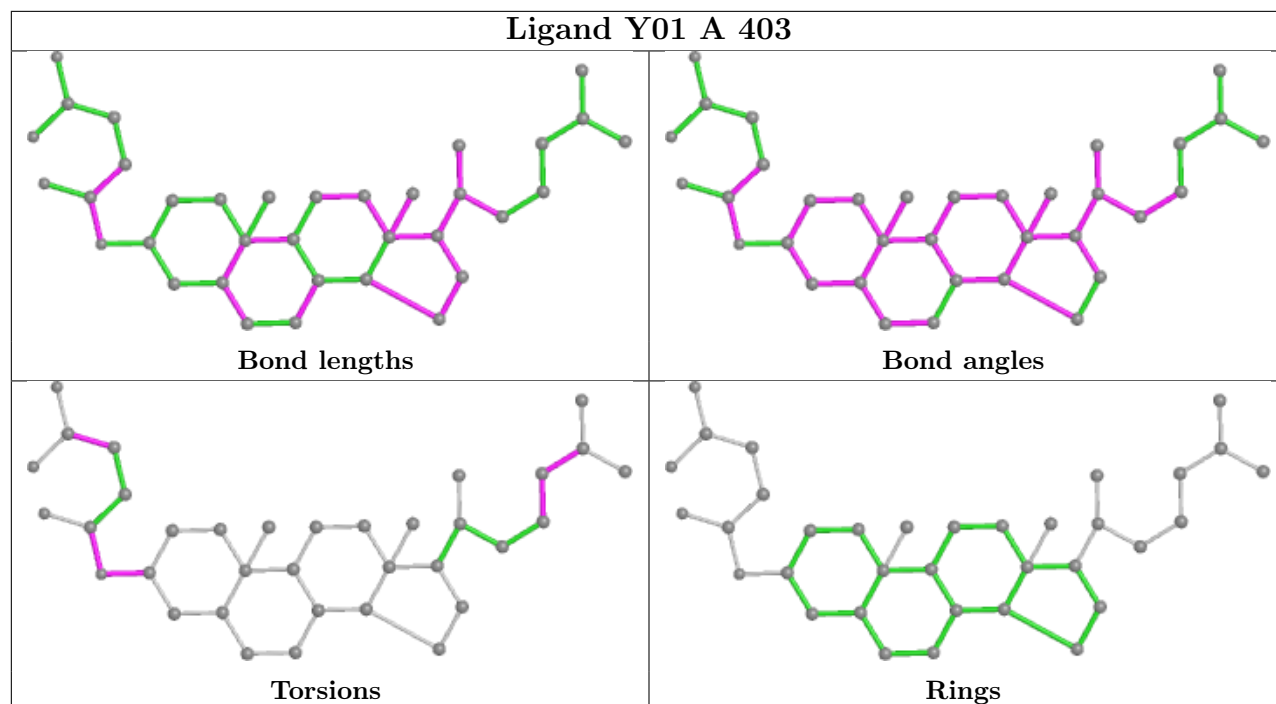
Mol	Chain	Res	Type	Atoms
6	B	402	Y01	CAL-CAM-CAY-OAW
6	A	404	Y01	CAM-CAL-CAX-OAF

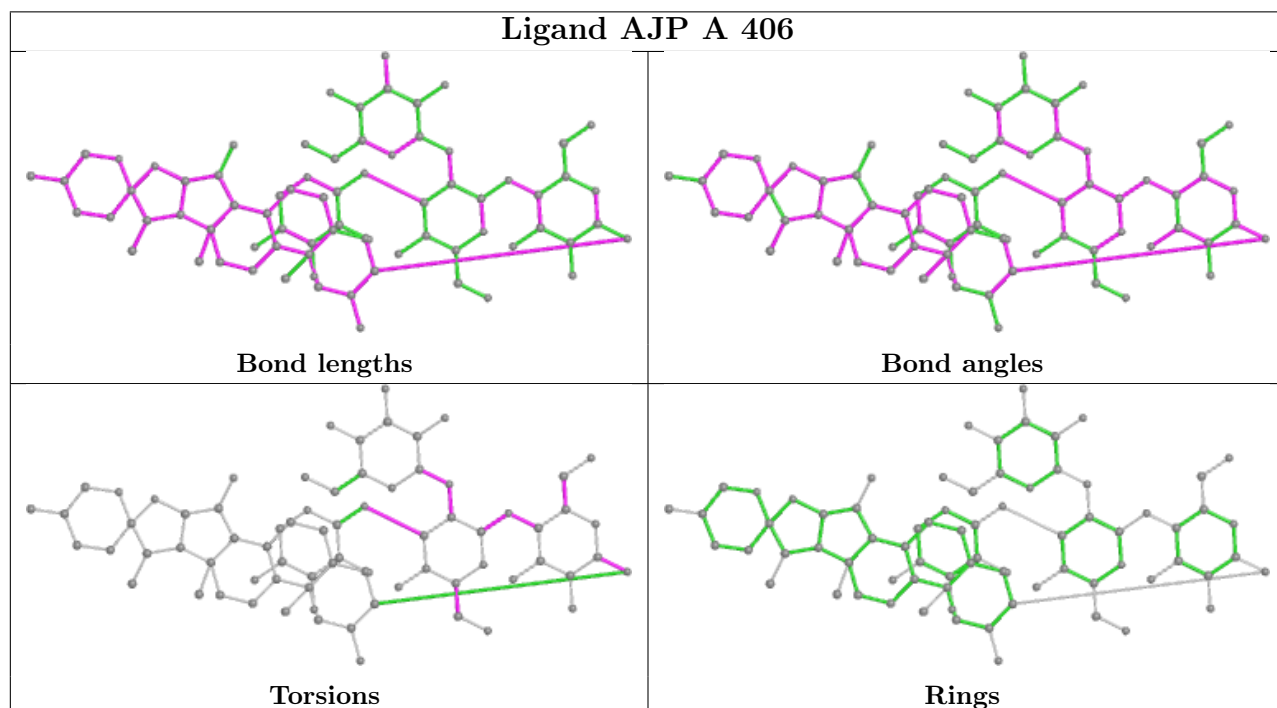
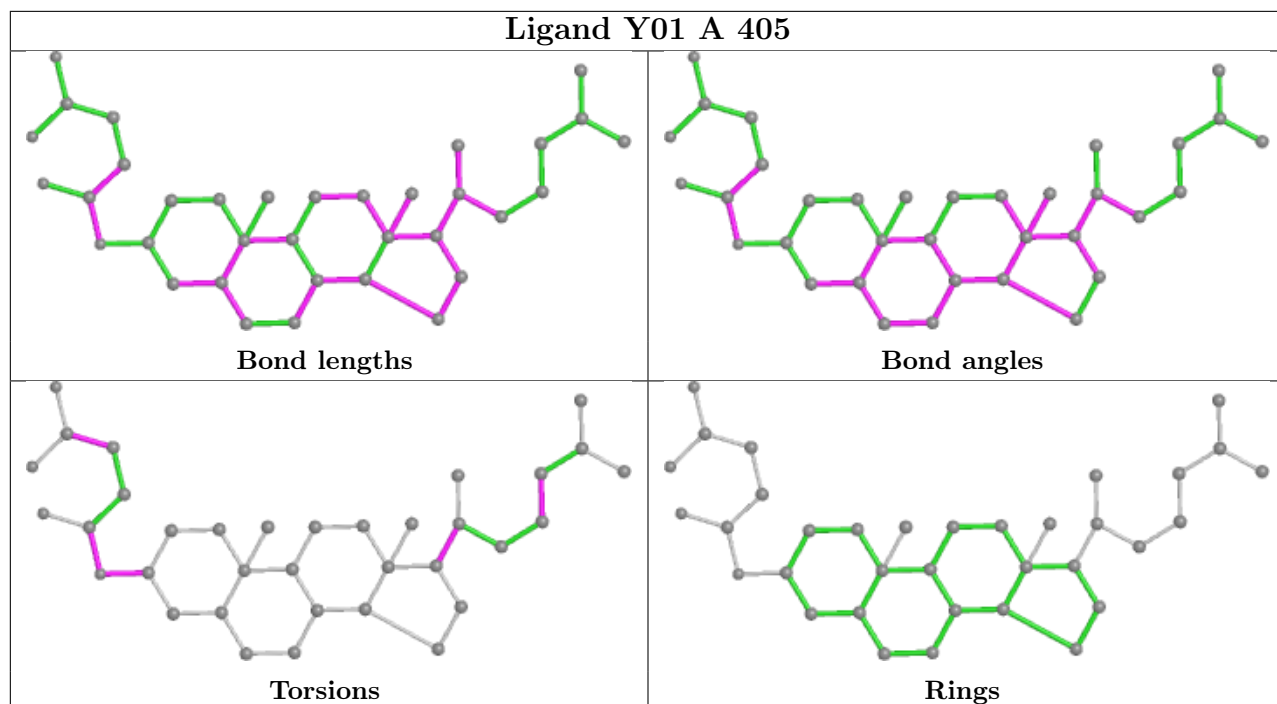
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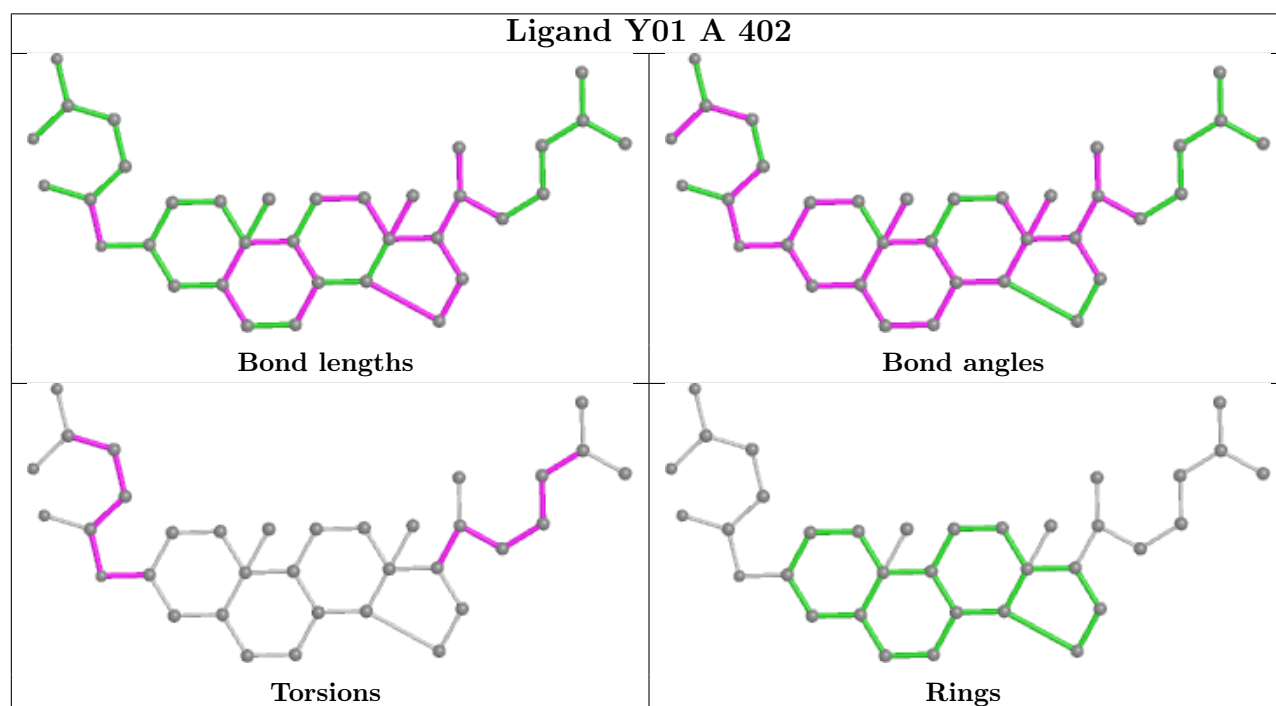
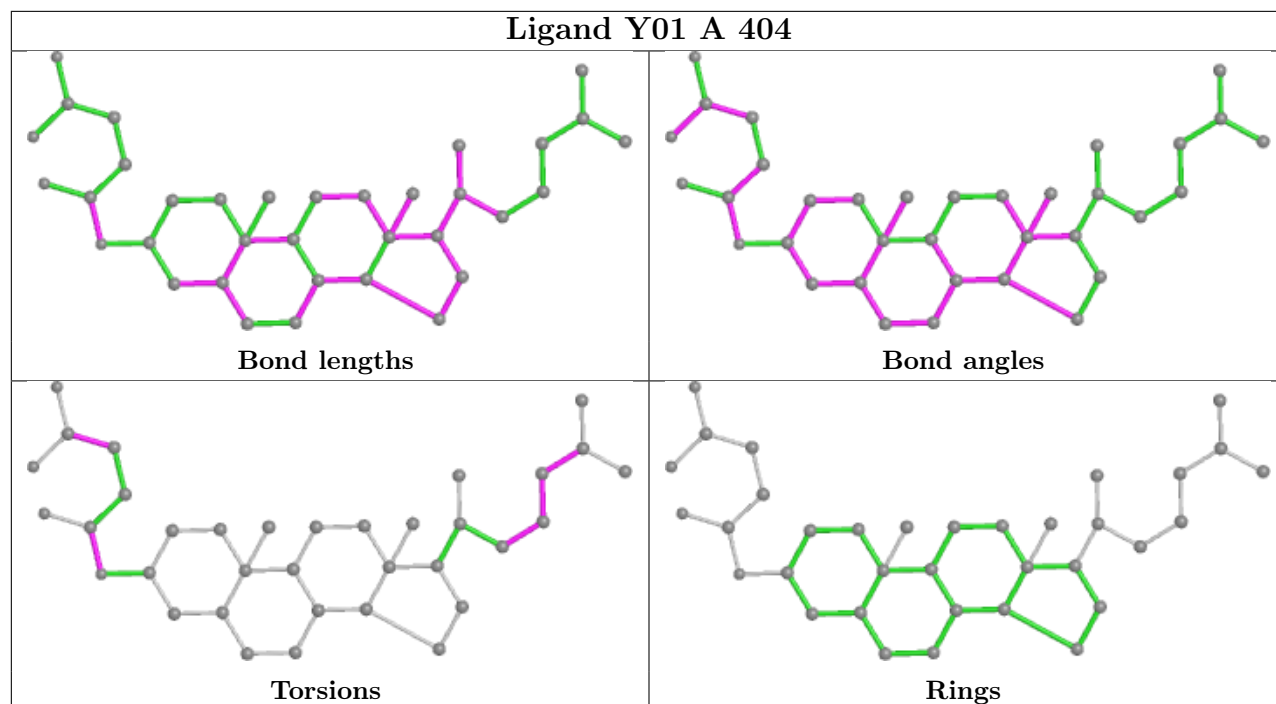
8 monomers are involved in 75 short contacts:

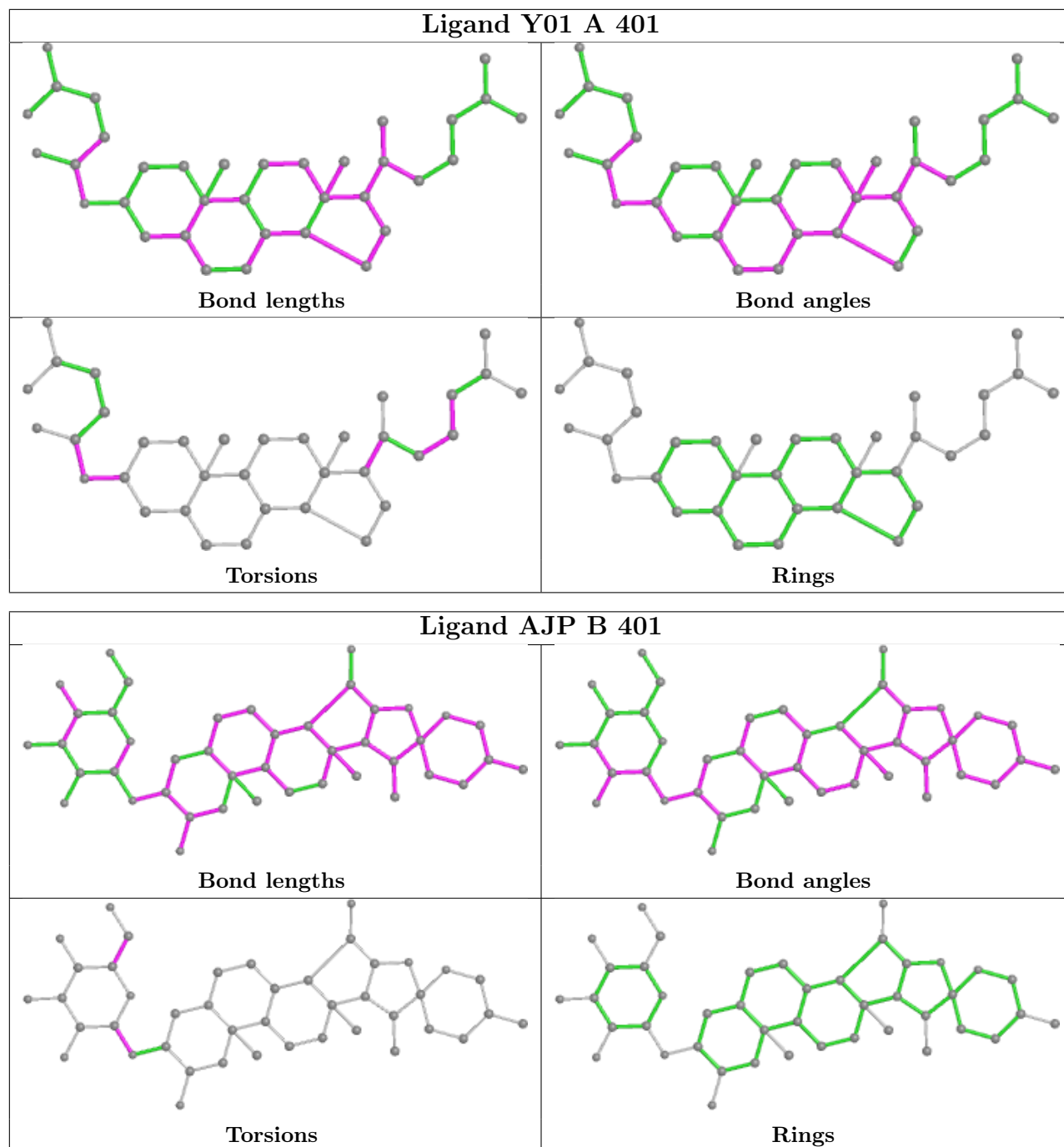
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	403	Y01	3	0
6	B	402	Y01	8	0
6	A	405	Y01	6	0
7	A	406	AJP	22	0
6	A	404	Y01	6	0
6	A	402	Y01	2	0
6	A	401	Y01	7	0
7	B	401	AJP	21	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

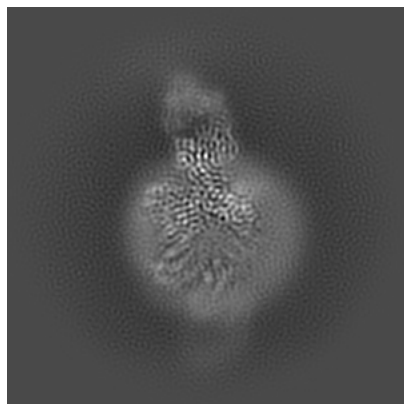
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27460. These allow visual inspection of the internal detail of the map and identification of artifacts.

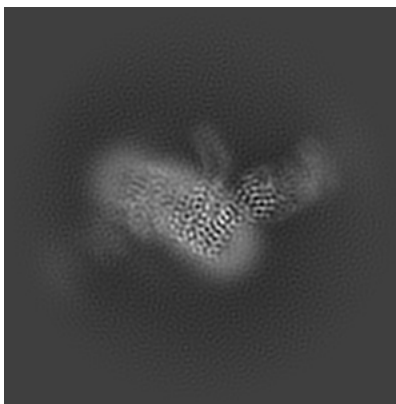
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

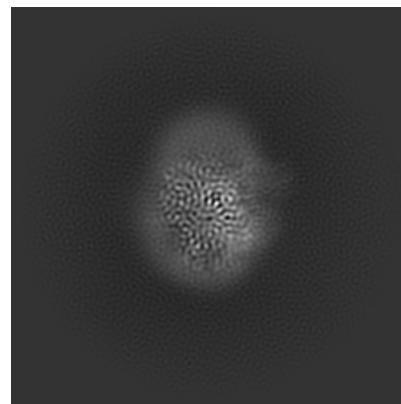
6.1.1 Primary map



X

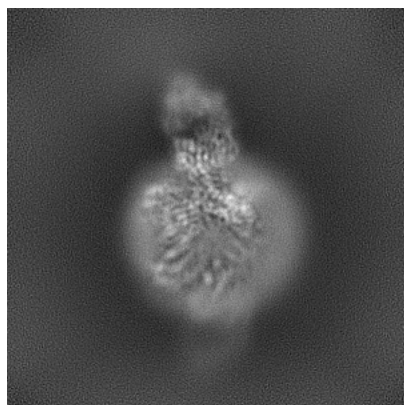


Y

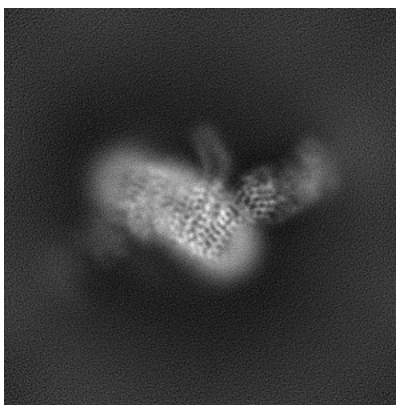


Z

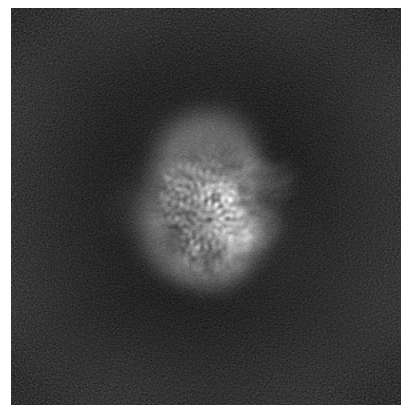
6.1.2 Raw map



X



Y

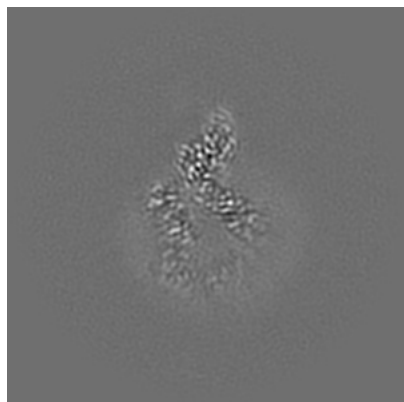


Z

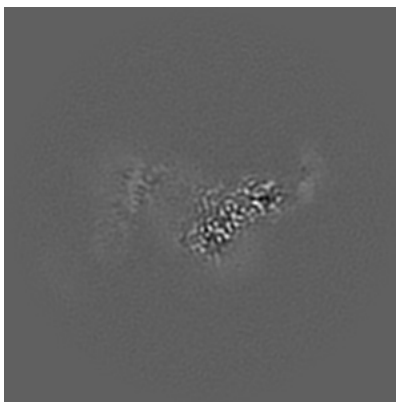
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

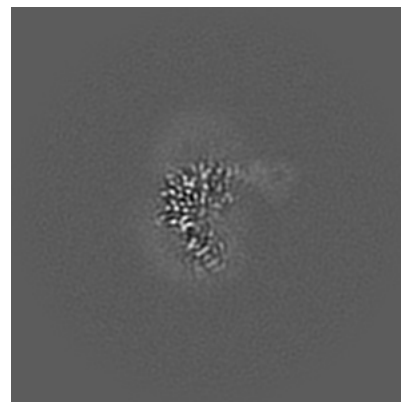
6.2.1 Primary map



X Index: 160

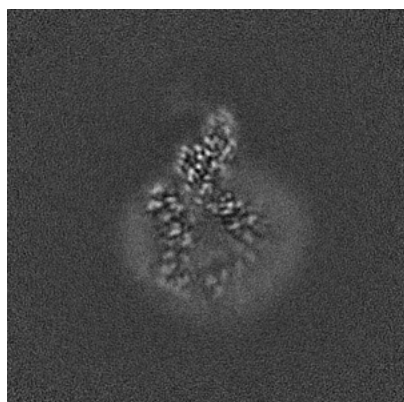


Y Index: 160

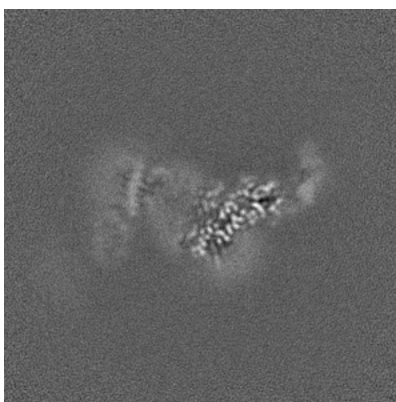


Z Index: 160

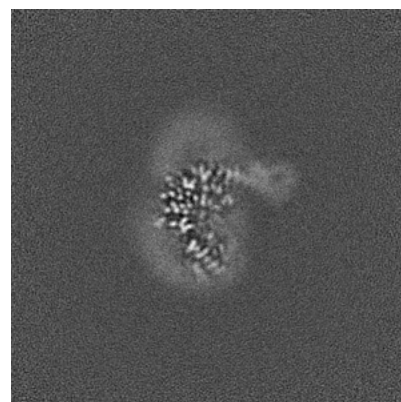
6.2.2 Raw map



X Index: 160



Y Index: 160

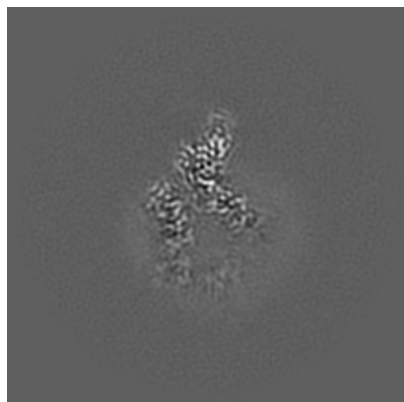


Z Index: 160

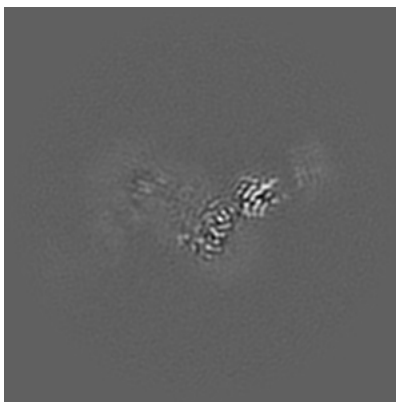
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

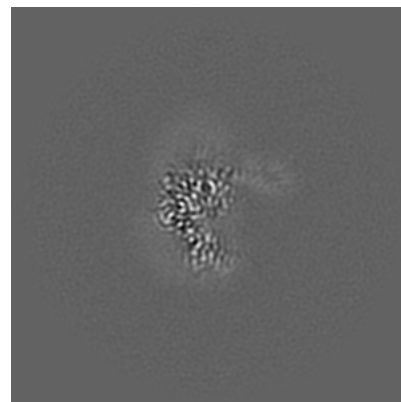
6.3.1 Primary map



X Index: 158

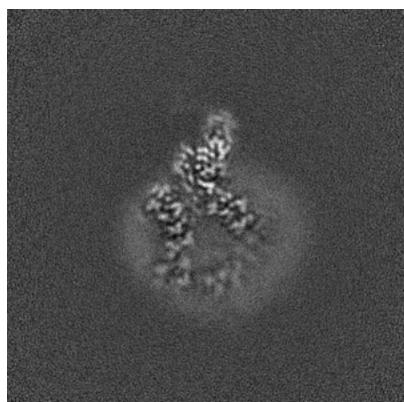


Y Index: 153

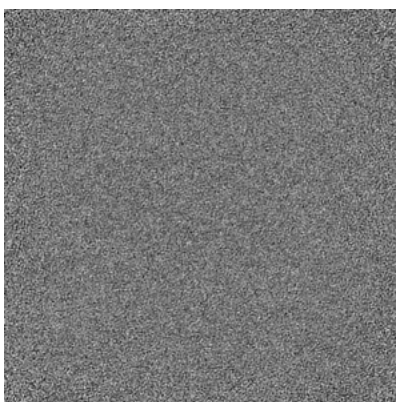


Z Index: 163

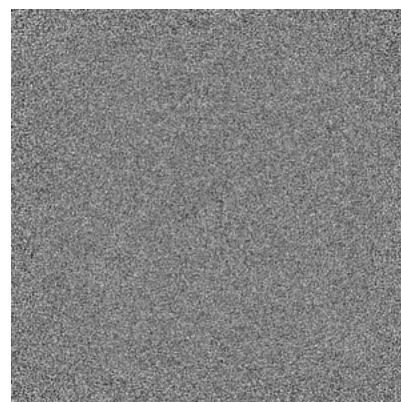
6.3.2 Raw map



X Index: 158



Y Index: 0

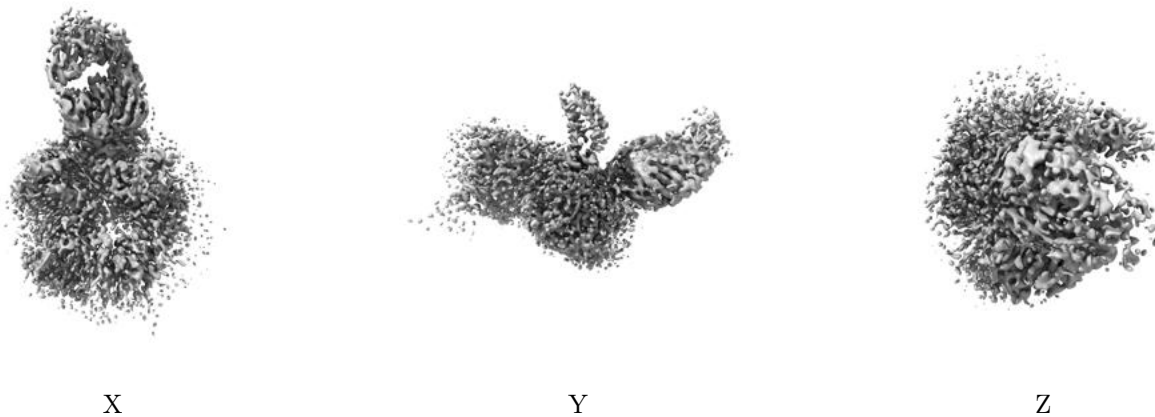


Z Index: 0

The images above show the largest variance slices of the map in three orthogonal directions.

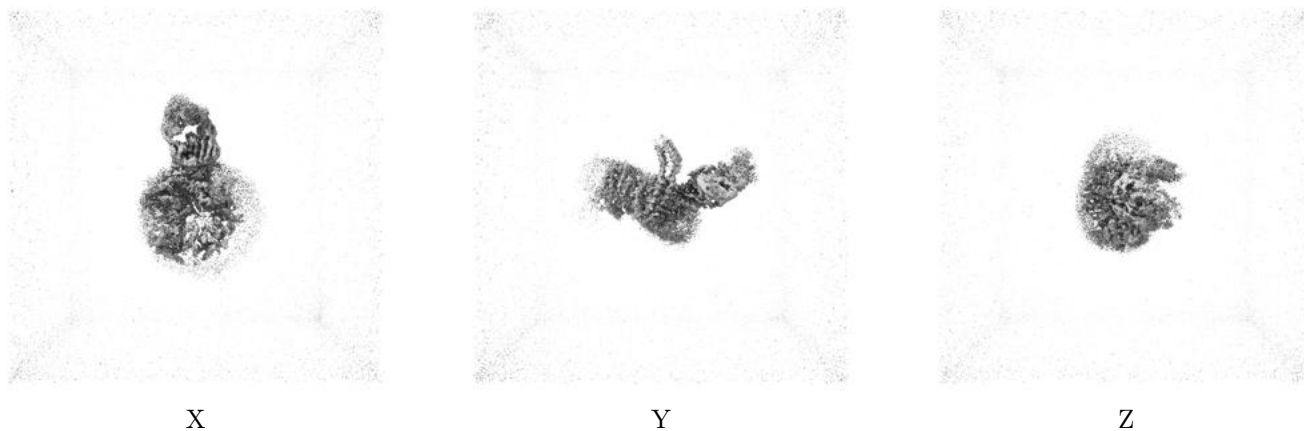
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.351. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

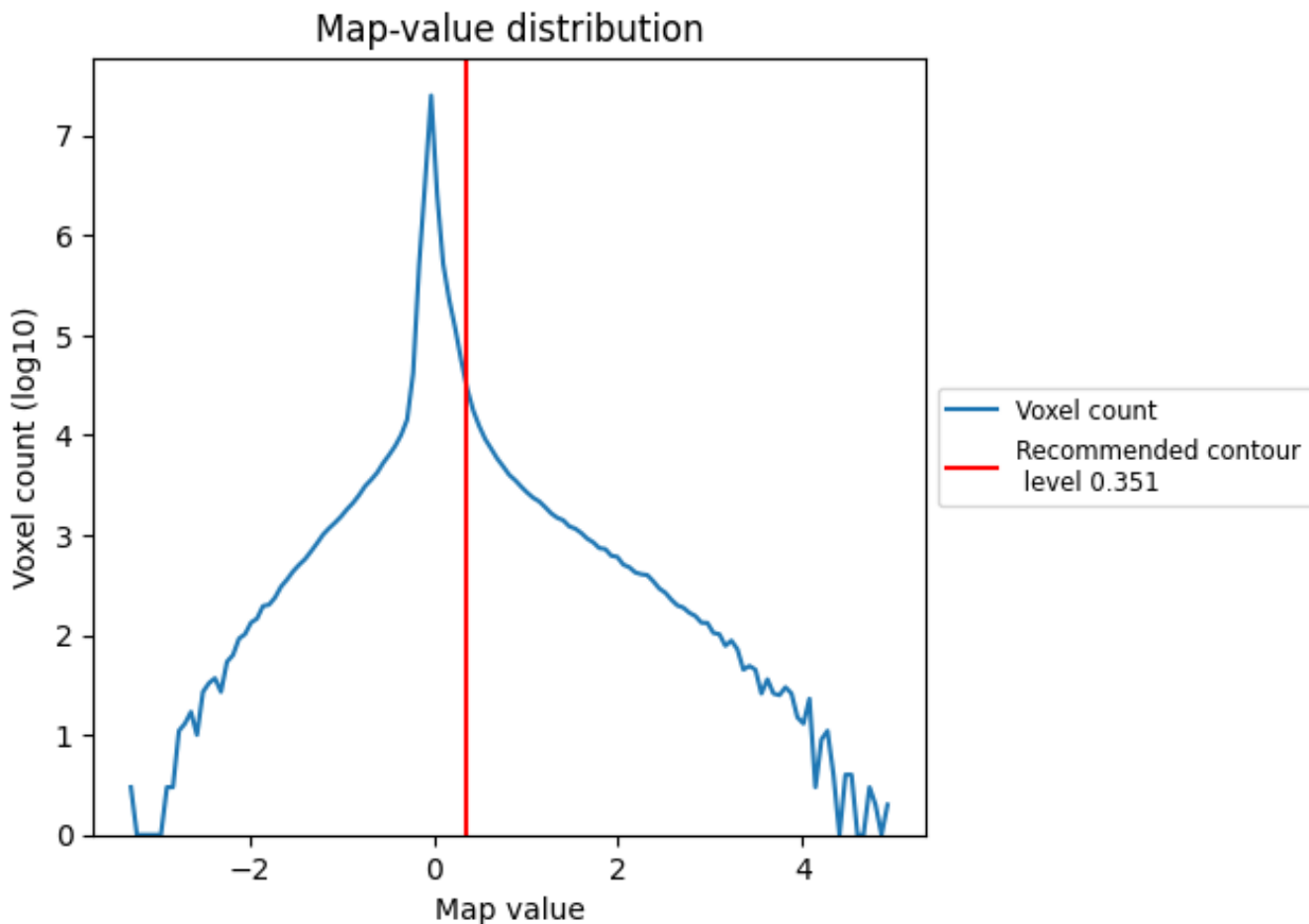
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

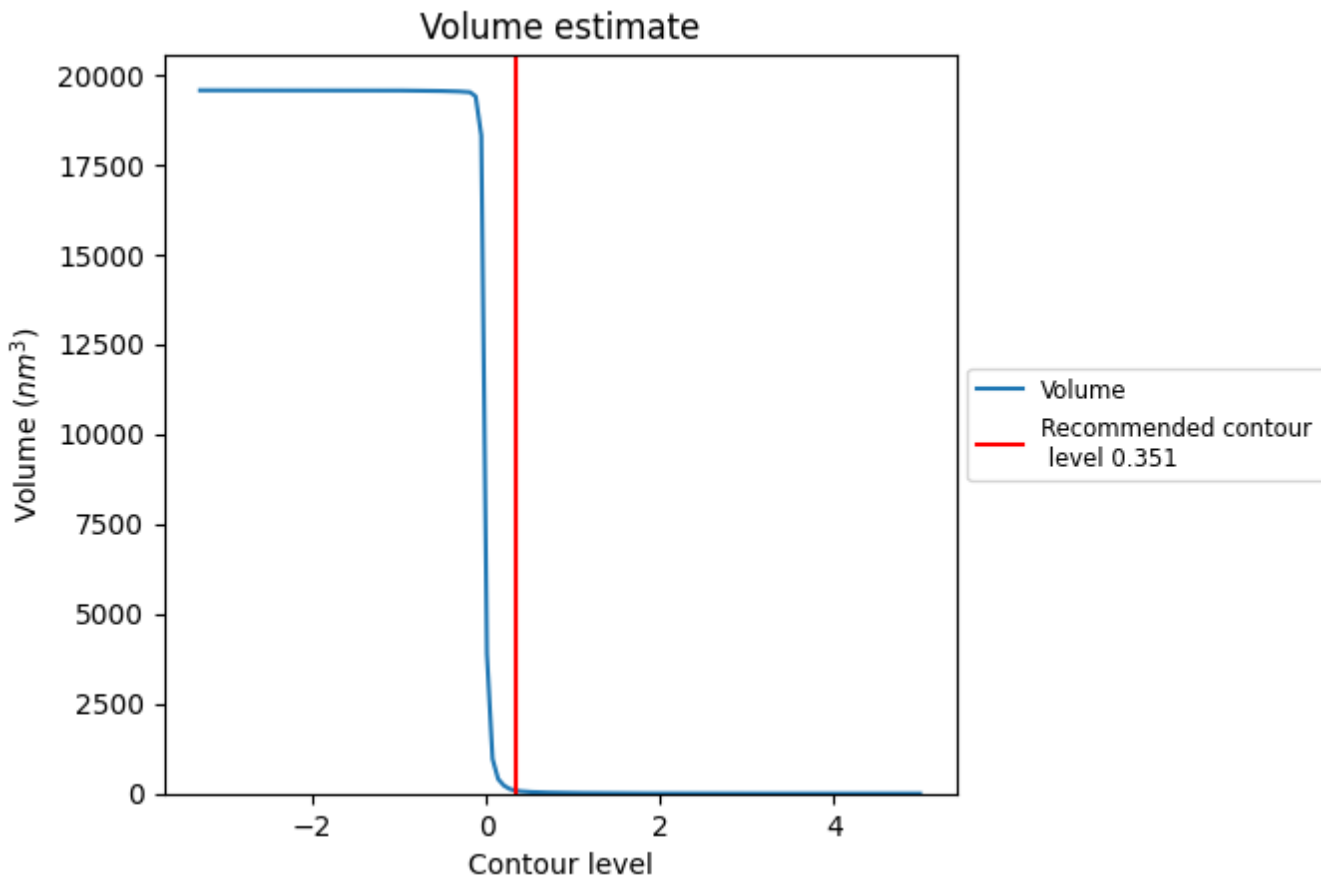
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

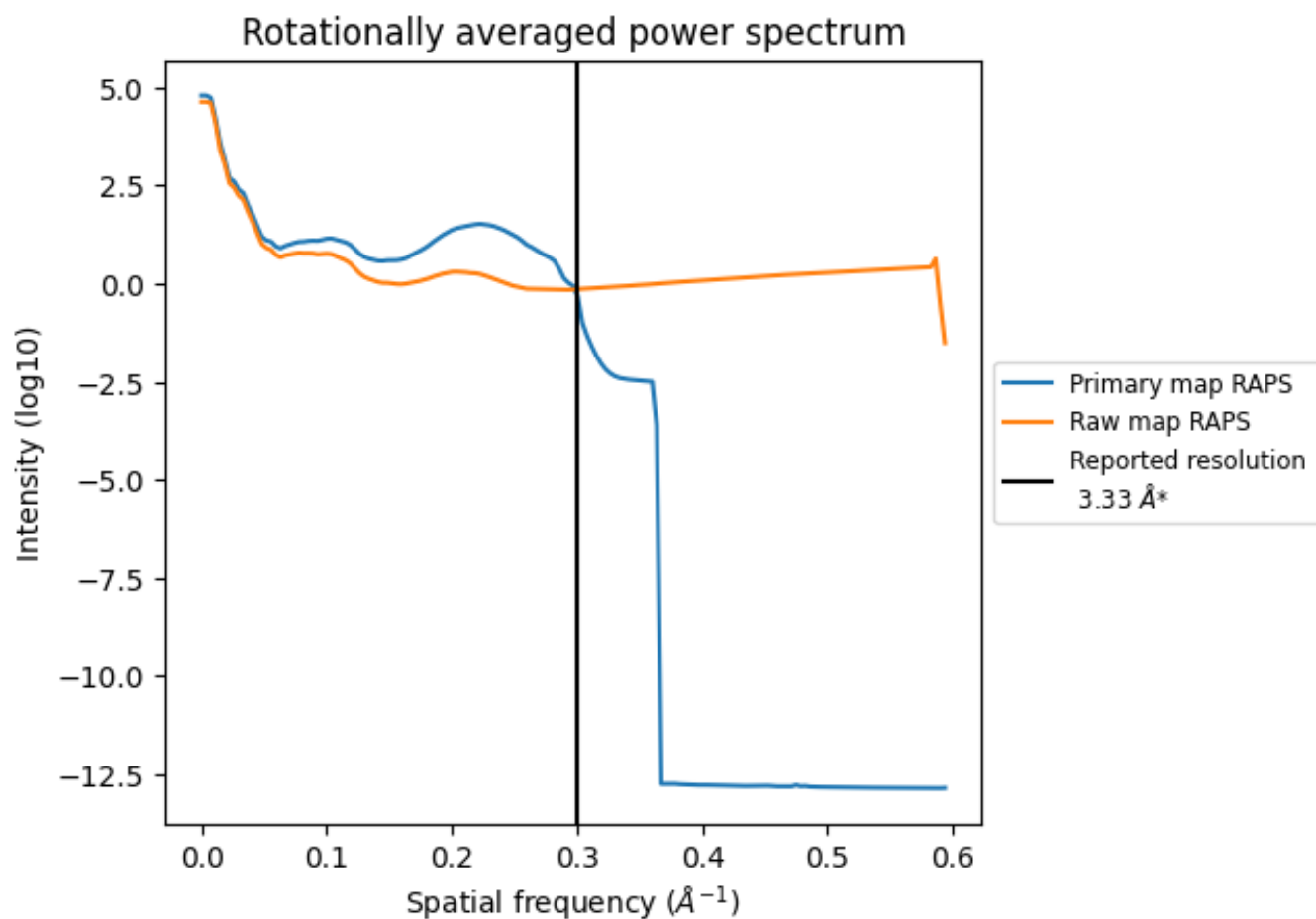
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm³; this corresponds to an approximate mass of 71 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

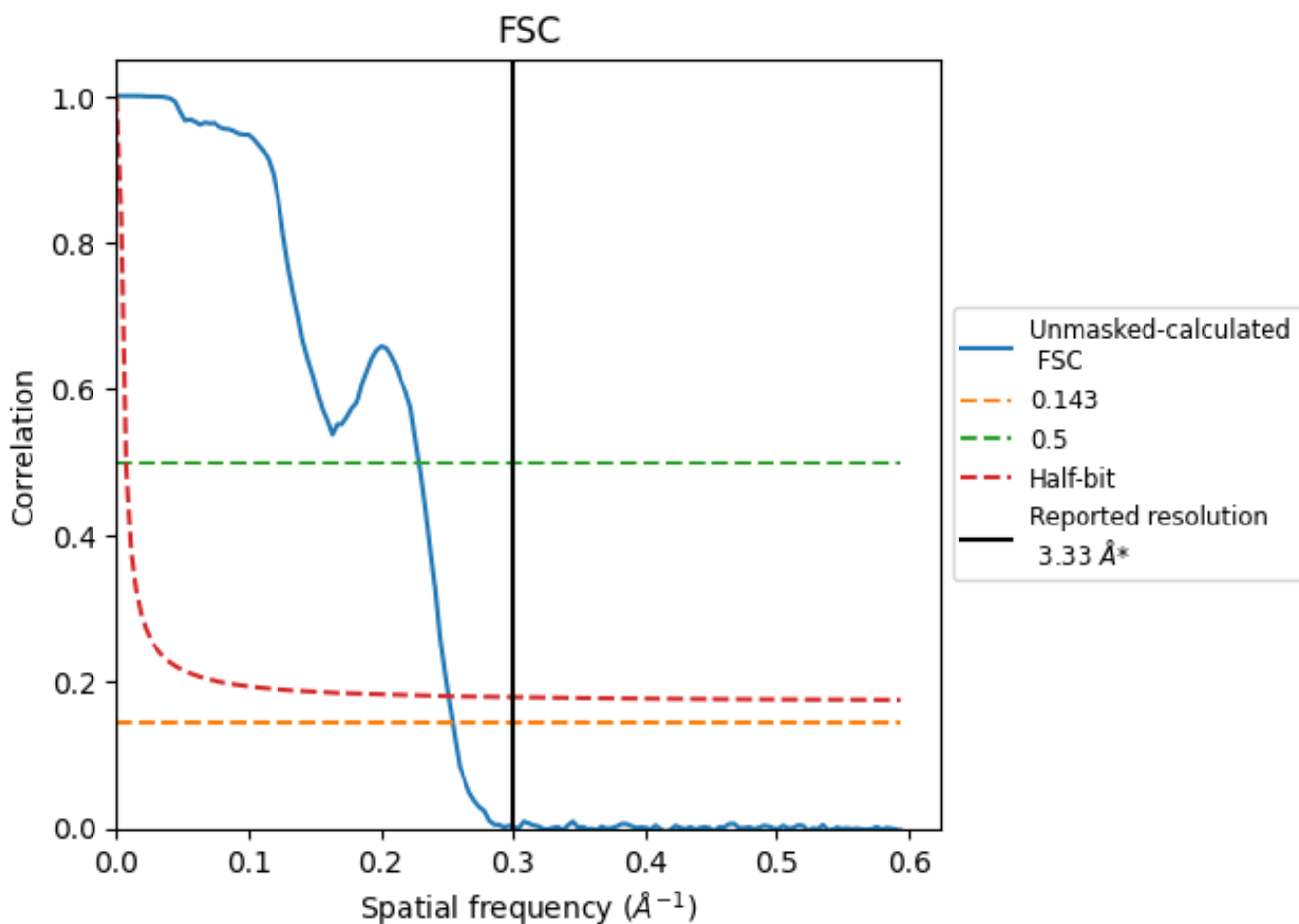


*Reported resolution corresponds to spatial frequency of 0.300 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 \AA^{-1}

8.2 Resolution estimates [i](#)

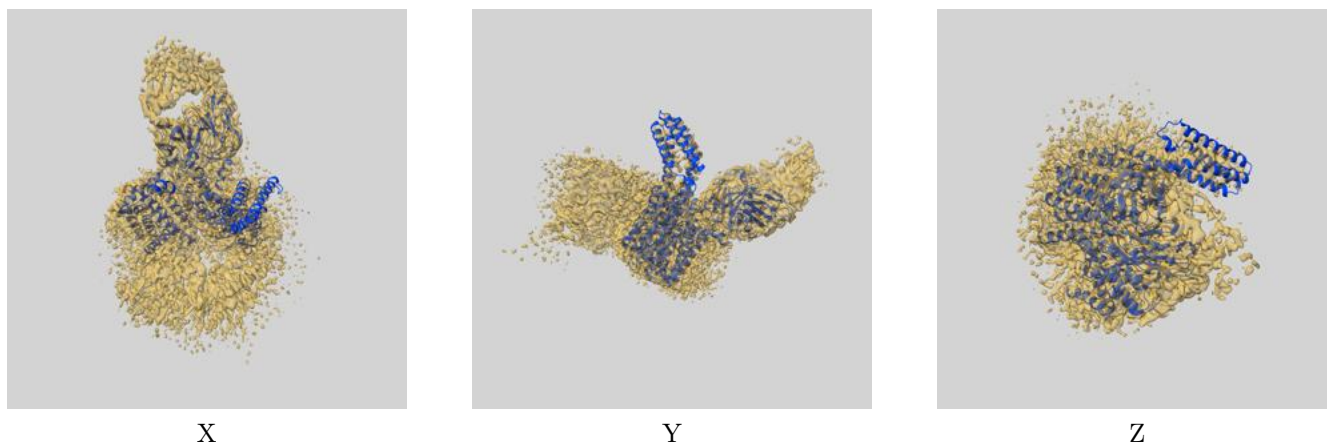
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	4.37	3.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

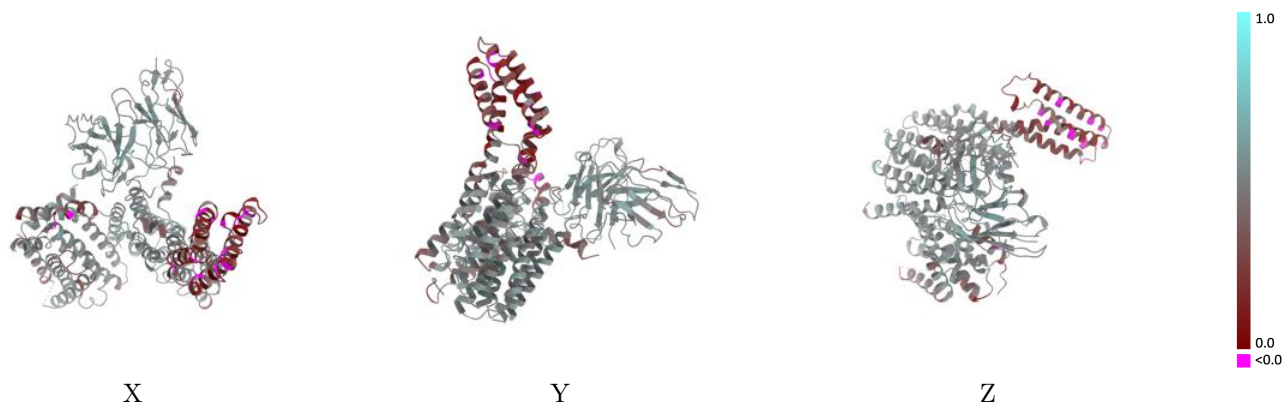
This section contains information regarding the fit between EMDB map EMD-27460 and PDB model 8DJK. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



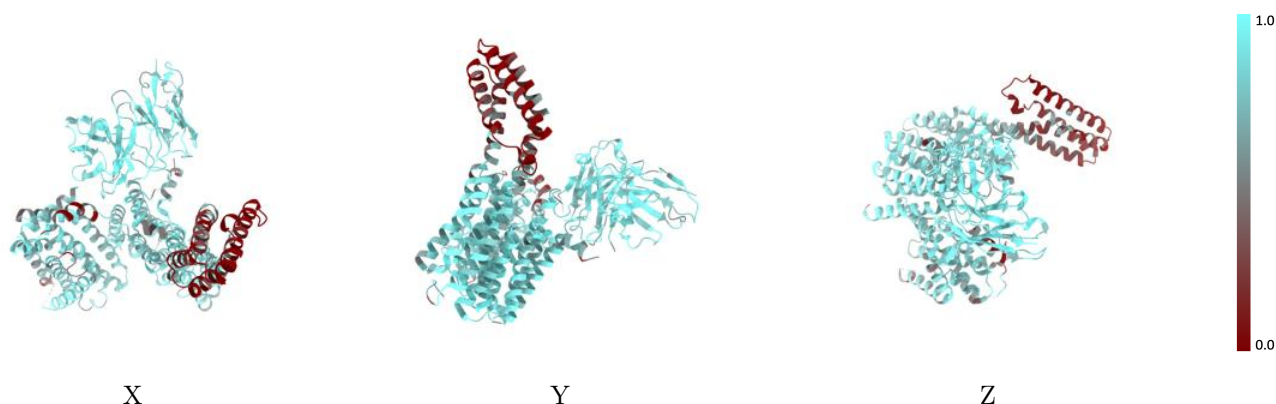
The images above show the 3D surface view of the map at the recommended contour level 0.351 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



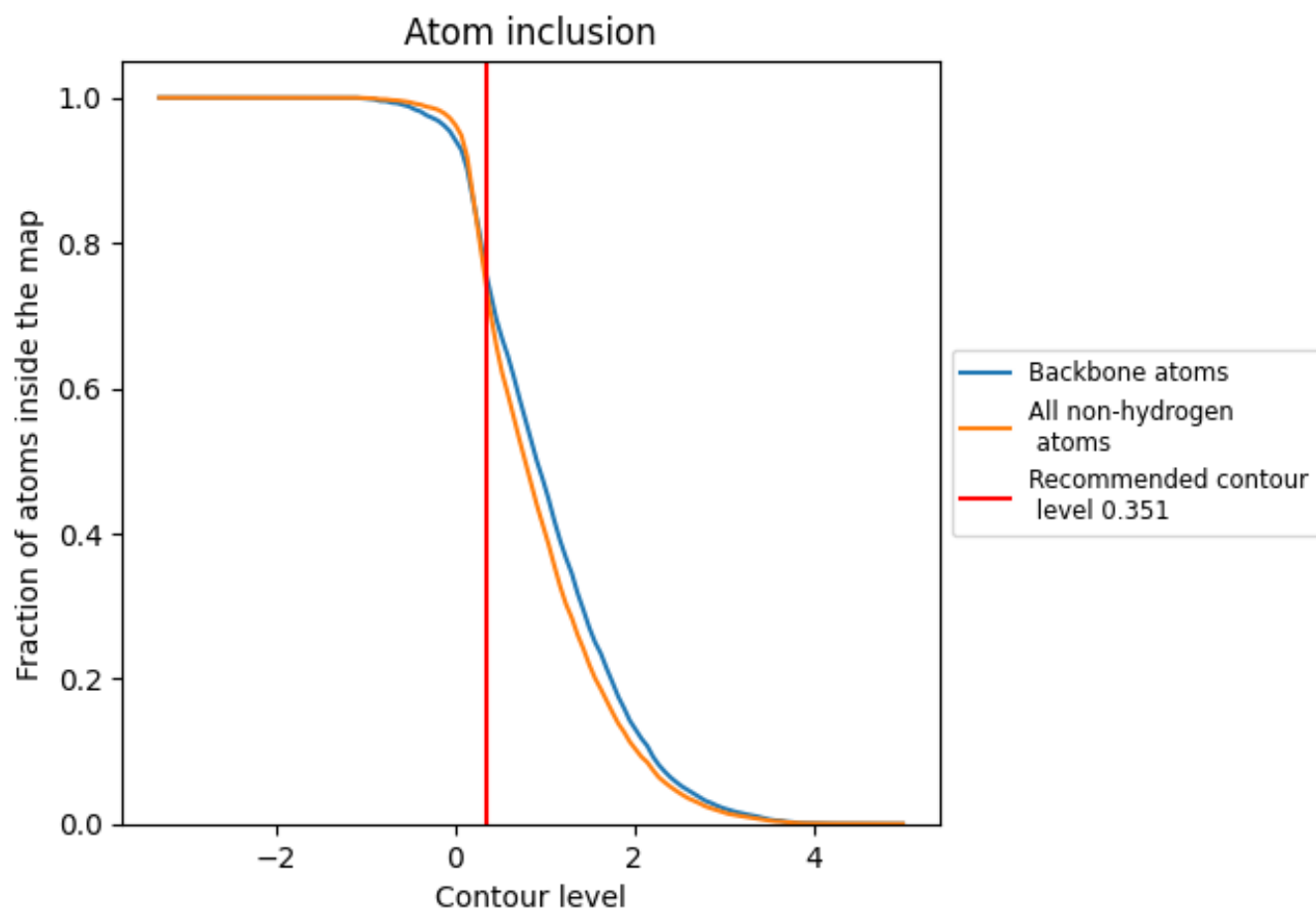
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.351).













9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.351) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7382	 0.4500
A	 0.7640	 0.4530
B	 0.8297	 0.4920
C	 0.2233	 0.2250
H	 0.8867	 0.5300
L	 0.8483	 0.4970

